SOLUTION OF SOME INITIAL-VALUE PROBLEMS FOR THE SEMI-INFINITE UNIFORM LINEAR CHAIN WITH FINITELY MANY DEFECTS

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SOLUTION OF SOME INITIAL-VALUE PROBLEMS

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LINEAR CHAIN WITH FINITELY MANY DEFECTS

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With the unfailing support of my wife, Valerie, this project has been completed. It is to her that I dedicate this dissertation.

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SUMMARY

This study reports the results of a mathematical investigation of semi-infinite uniform linear chains with finitely many defects. A physical system which the mathematics describes is a one-dimensional mechanical array of coupled harmonic oscillators extending indefinitely in one direction only. All but a finite number of the inertial elements and all but a finite number of the elastic elements in the array are alike.

An explicit solution of a basic initial-value problem associated with the equations of motion of any semi-infinite harmonic chain with nearest-neighbor coupling is provided by an integral representation of A. G. Law (Doctoral Dissertation, Georgia Institute of Technology, 1968). Use of this representation for a given problem requires explicit knowledge of a suitable sequence of orthogonal polynomials and a distribution associated with them. The polynomials are generated by a three-term recurrence relation obtained directly from the equations of motion of the chain, but the distribution must be constructed.

The principal result of the present study is a procedure for constructing the distribution needed in solving initial-value problems for semi-infinite linear chains which are uniform except for a finite number of defects. Defects which are referred to in the physics literature as isotopes, holes, and interstitials are interpreted here as defects in a semi-infinite uniform chain. The resulting mechanical

systems are special cases of the systems under investigation, and construction of the distributions appropriate to these cases is considered in some detail.

CHAPTER I

INTRODUCTION

Physical systems in which most of the elements are prescribed according to a regular pattern are said to contain defects if some of the elements fail to conform to the pattern. The mathematical analysis of such systems is an area of active current investigation, where questions in the theory of the dynamics of atomic lattices are of particular interest [14]. The purpose of this presentation is to report the results of a mathematical study of one class of such problems--the semi-infinite uniform linear chain with *finitely* many defects.

The mathematics of this investigation is phrased in terms of a mechanical system consisting of a one-dimensional array of coupled harmonic oscillators extending to infinity in one direction only. All but a finite number of the elements in the array are alike. In the absence of frictional forces, the equations of motion comprise a countable system of ordinary differential equations of the form $X''(t) = AX(t)$, where X is an infinite column vector and A is an infinite tridiagonal matrix of constants. All except finitely many elements in the main diagonal of A are alike, and similar statements may be made for the elements in the first subdiagonal and the first superdiagonal. Explicit representations of solutions of some initial-value problems involving this differential system are obtained by using an integral representation derived by A. G. Law [13].

In applying Law's representation, use is made of a sequence of orthogonal polynomials generated by a three-term recurrence obtained directly from the differential equations, and a distribution with respect to which the polynomials are orthogonal is determined. The procedure used to derive this distribution is motivated by results of W. F. Martens [15] for a special case of the problem considered here. Parenthetically, it may be noted that the procedure is also applicable to the solution of some other infinite linear differential systems involving a finite number of perturbations of the coefficients [12,13, 15].

The lattice defects referred to in the physics literature as isotopes, holes, and interstitials are interpreted here as defects in a semi-infinite uniform chain. The resulting mechanical systems are special cases of the systems under investigation, and construction of the distributions appropriate to these special cases is considered in some detail.

The discussion in Chapter I is primarily for orientation. In Chapter II the isotope, hole, and interstitial for semi-infinite linear chains are introduced and are used to motivate consideration of the semi-infinite uniform linear chain with finitely many defects. Then a statement is given of the basic initial-value problem [IVP] to be solved.

Some nomenclature and results related to the study of orthogonal polynomials are given in Chapter III. Then the connection between recursively generated orthogonal polynomials and the solution of [IVP] is established by way of Law's integral representation, thereby reducing the problem of solving [IVP] to the problem of finding a distribution for the sequence $\{R_n(x)\}$ of orthogonal polynomials generated by

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_{n+1}(x) = (2a_n x+b_n)R_n(x) - c_n R_{n-1}(x), \quad 0 \leq n \leq N-1,$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad n \geq N,$$

where N is a fixed nonnegative integer.

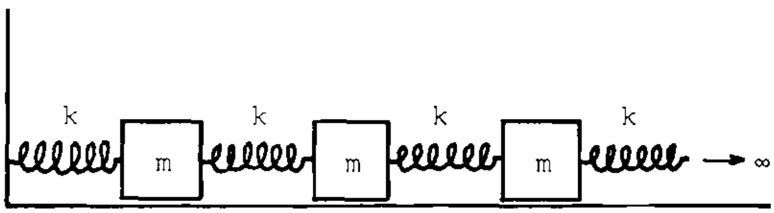
Chapter IV deals with this reduced problem. Section 1 of Chapter IV gives an outline of a procedure for constructing a distribution function α_R such that $\{R_n(x)\}$ is orthogonal with respect to the distribution $d\alpha_R(x)$. α_R is a real-valued, bounded, non-decreasing function on $(-\infty,\infty)$ which assumes infinitely many different values. By Theorem 4.5, the main result of Chapter IV, α_R is represented as the sum of two non-decreasing functions α_1 and α_2, where α_1 is an absolutely continuous distribution function on $[-1,1]$ and α_2 is a step function with finitely many jumps, all outside $[-1,1]$. The weight function associated with $d\alpha_1(x)$ is $\frac{2\sqrt{1-x^2}}{\pi S(x)}$ on $[-1,1]$, where $S(x)$ is a polynomial. The location of the jumps in α_2, the amount of these jumps, and the polynomial $S(x)$ are determined from knowledge of a polynomial $P(z)$ derivable from the recurrence relation. Sections 2-5 of Chapter IV are concerned with the proof of Theorem 4.5. Some representations of $\{R_n(x)\}$ useful in the application of Theorem 4.5 are contained in section 2. Normalization of the distribution $d\alpha_R(x)$ is discussed in section 6.

In Chapter V the distribution constructed in the preceding chapter is used to develop a general formula (Theorem 5.1) for the solution of [IVP]. A result of W. G. Christian [8] aids in this development. The single isotope, single hole, and single interstitial are then discussed as examples. Chapter VI treats these special cases for the semi-infinite chain which is not attached by a spring to the inertial system.

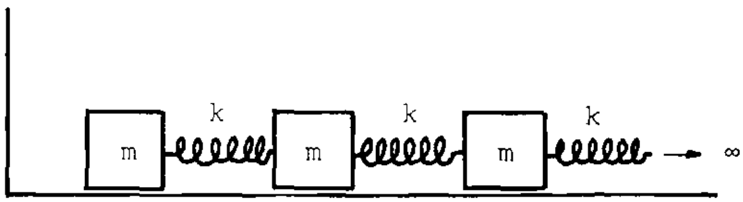
CHAPTER II

THE BASIC INITIAL-VALUE PROBLEM FOR THE FINITELY DEFECTIVE CHAIN

Consider a semi-infinite chain of particles (masses) and linear springs in which every particle has the same mass, say m, and every spring has the same spring constant, say k (Figure 1).



(a) Chain with Initial Spring



(b) Chain without Initial Spring

Figure 1. Uniform Semi-Infinite Chains

Such a chain is said to be *uniform*. Introducing *defects* into a uniform chain consists of removing or changing the masses of some of the particles and/or changing the spring constants of some of the springs. It is understood that the chain is not to be severed, except perhaps from the inertial system (thus any semi-infinite chain without the initial spring--even a uniform one--can be thought of as a chain of the type shown in Figure 1(a) into which defects have been introduced).

Some of the isolated defects frequently discussed in connection with the theory of lattice dynamics [16] are now interpreted as defects in a semi-infinite (uniform) chain of particles and masses of the type depicted in Figure 1(a).

(i) *Impurity*--replacement of a particle in the chain by another particle of mass m', with an accompanying change (say from k to k') in the spring constants of the connecting springs (Figure 2).

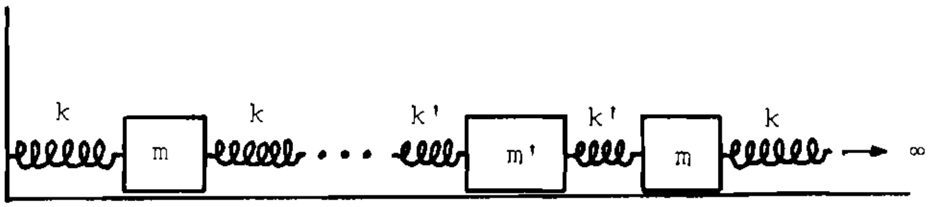
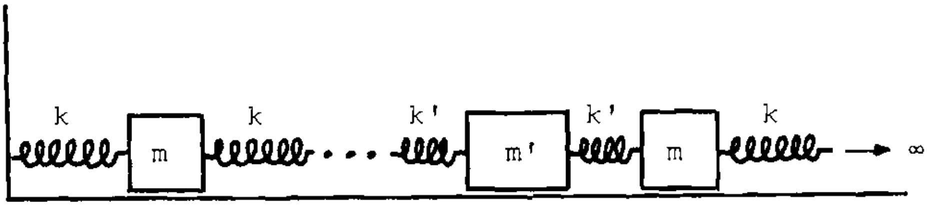
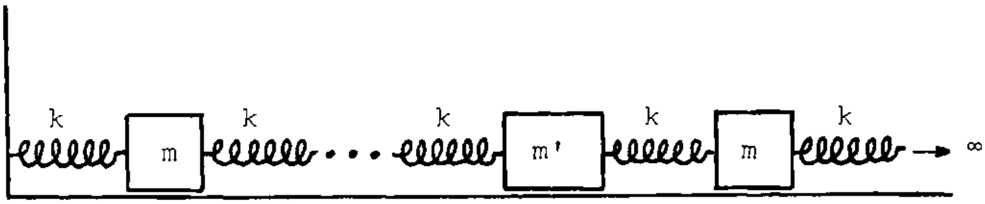


Figure 2. Uniform Semi-Infinite Chain with an Isolated Impurity

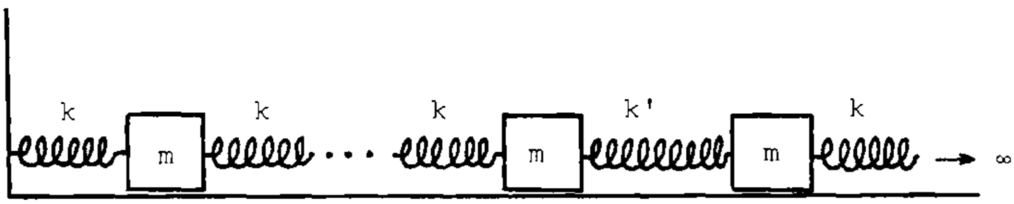
(ii) *Interstitial*--insertion of a particle of mass m' between two other particles. This can be visualized to have taken place by first removing one of the springs and then inserting the new mass together with connecting springs (with spring constants k') in the position of the removed spring (Figure 3(a)) (note that in the one-dimensional semi-infinite case the interstitial and the impurity are mathematically equivalent).



(a) Interstitial



(b) Isotope



(c) Hole

Figure 3. Uniform Semi-Infinite Chains with Isolated Defects

(iii) *Isotope*--replacement of a particle by another particle with mass m' *without* an accompanying change of spring constants (Figure 3(b)).

(iv) *Hole*--removal of a particle from the chain with an accompanying change (from k to k') in the spring constants of the previously connecting springs. Mathematically (for the semi-infinite chain) this is the same as changing one of the spring constants (Figure 3(c)).

Now consider a semi-infinite uniform chain (with initial spring) into which finitely many defects of the type described above have been introduced. Let N be the smallest nonnegative integer such that there are no defects to the right of the N*th* mass (thus $N = 0$ corresponds to the uniform chain). The resulting chain is depicted in Figure 4, where some of the factors λ_i and μ_i $(0 \le i \le N-1)$ may be equal to 1; where λ_0 may be zero, but $\lambda_i > 0$ $(1 \le i \le N-1)$; and where $\mu_i > 0$ $(0 \le i \le N-1)$. In this presentation such a chain is called *finitely defective*. The problem to be investigated is now stated.

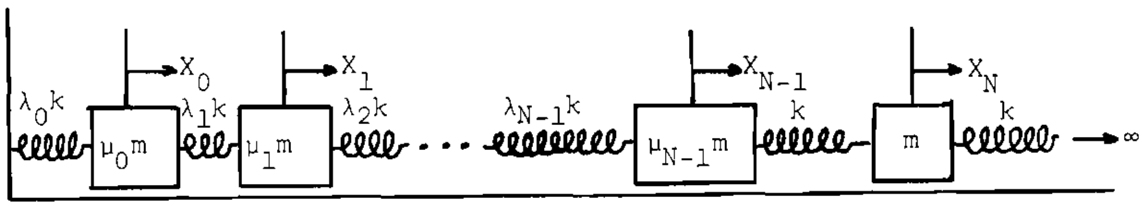


Figure 4. The Finitely Defective Semi-Infinite Chain $(N \ge 1)$

Problem I. Consider the finitely defective semi-infinite chain of springs and masses (Figure 4) in which friction of all types is assumed to be negligible. Given finitely many nonzero initial displacements and finitely many nonzero initial velocities for the masses, determine the displacements $X_n(t)$ $(n \ge 0, t \ge 0)$.

In mathematical terms, a solution is desired for the initial-value problem consisting of the appropriate equations of motion for the masses together with initial conditions of the type

$$X_{r_i}(0) = d_i, \quad X_n(0) = 0, \quad n \neq r_i \ (1 \leq i \leq I),$$
$$X'_{s_j}(0) = v_j, \quad X'_n(0) = 0, \quad n \neq s_j \ (1 \leq j \leq J), \qquad \text{[IC1]}$$

where I and J are fixed nonnegative integers.

The equations of motion are

$$\mu_0 m X''_0(t) = -\lambda_0 k X_0(t) + \lambda_1 k[X_1(t) - X_0(t)],$$

$$\mu_n m X''_n(t) = -\lambda_n k[X_n(t) - X_{n-1}(t)] + \lambda_{n+1} k[X_{n+1}(t) - X_n(t)], \quad 1 \leq n \leq N-1,$$

$$m X''_n(t) = -k[X_n(t) - X_{n-1}(t)] + k[X_{n+1}(t) - X_n(t)], \quad n \geq N,$$

where $\lambda_N \stackrel{d}{=} 1$. It will be convenient later to have this system written in the form

$$-\frac{\mu_0 m}{\lambda_1 k} X''_0(t) = \left(1 + \frac{\lambda_0}{\lambda_1}\right) X_0(t) - X_1(t),$$

$$-\frac{\mu_n m}{\lambda_{n+1} k} X''_n(t) = -\frac{\lambda_n}{\lambda_{n+1}} X_{n-1}(t) + \left(1 + \frac{\lambda_n}{\lambda_{n+1}}\right) X_n(t) - X_{n+1}(t), \quad 1 \leq n \leq N-1, \qquad \text{[DE]}$$

$$-\frac{m}{k} X''_n(t) = -X_{n-1}(t) + 2X_n(t) - X_{n+1}(t), \quad n \geq N,$$

where $\lambda_N \stackrel{d}{=} 1$. If a solution of [DE] subject to the initial conditions

$$X_n(0) = X_n'(0) = 0, \quad n \neq r$$

$$X_r(0) = d_r, \quad X_r'(0) = v_r \qquad \text{[IC2]}$$

were known for all $r \geq 0$, then Problem I could be solved by superposition of such solutions. Let [IVP] be the initial-value problem consisting of [DE] and [IC2]. The purpose of this study, then, is to find a solution of [IVP].

CHAPTER III

THE ROLE OF ORTHOGONAL POLYNOMIALS IN THE SOLUTION OF THE BASIC INITIAL-VALUE PROBLEM

In this chapter it will be seen that the problem of solving [IVP] can be reduced, by way of an integral representation given by A. G. Law [13], to the problem of finding a distribution (see definition below) for an associated sequence of orthogonal polynomials. Some of the nomenclature and results which accompany this development are given first.

Definition 3.1. A *distribution function* α is a real-valued, bounded, non-decreasing function on $(-\infty,\infty)$ such that α assumes infinitely many different values.

Definition 3.2. Let α be a distribution function. Then α induces a Lebesgue-Stieltjes measure on a class of subsets of the real line. This measure is called the *distribution* $d\alpha(x)$.

Thus $\int_{-\infty}^{x} d\alpha(y)$ can be thought of as the "mass" distributed over the real interval $(-\infty,x]$. Notice that since α is bounded,

$$\int_{-\infty}^{\infty} d\alpha(y) < \infty.$$

Definition 3.3. Let α be a distribution function satisfying

$$\lim_{x \to -\infty} \alpha(x) = 0$$

and

$$\int_{-\infty}^{\infty} d\alpha(x) = 1.$$

Then $d\alpha(x)$ is said to be a *normalized* distribution.

It should be noted that a normalized distribution can be obtained from any distribution function. For suppose that α_1 is a distribution function such that $\lim_{x \to -\infty} \alpha_1(x) = c_1$ and $\infty > \int_{-\infty}^{\infty} d\alpha_1(x) = c_2 > 0$. Let α be given by

$$\alpha(x) = \frac{1}{c_2}[\alpha_1(x) - c_1], \quad \text{all } x.$$

Then α is a distribution function, and $d\alpha(x)$ is a normalized distribution.

Definition 3.4. Let f be a real-valued function defined on $(-\infty, \infty)$. If $f(x_2) > f(x_1)$ for every x_1, x_2 satisfying $x_1 < x_0 < x_2$ in some neighborhood of x_0, then x_0 is called a *point of increase* of f.

Definition 3.5. Let α be a distribution function. The *support* of the distribution $d\alpha(x)$ is the set of points of increase of α.

If α is a distribution function, it can be shown that the support of $d\alpha(x)$ is a closed, infinite subset of the real line.

Definition 3.6. Let α be a distribution function, and let $[a,b]$ be a real interval (not necessarily bounded). If α is absolutely continuous on $[a,b]$, the distribution $d\alpha(x)$ can be represented by $w(x)dx$ over $[a,b]$, where w is nonnegative-valued and measurable. If $\int_a^b d\alpha(x) = \int_a^b w(x)dx > 0$, w is called a *weight function*, and one says that the distribution $d\alpha(x)$ is *given by the weight function w over $[a,b]$.*

Even if a distribution function α is not absolutely continuous on $(-\infty,\infty)$ it is convenient in some cases to think of $d\alpha(x)$ as $w(x)dx$ over $(-\infty,\infty)$, where w is a *generalized* weight function* (in the sense of Schwartz [20]). Then a corresponding interpretation of the integral must be made.

Definition 3.7. Let $\{P_n(x):\ n=0,1,\cdots\}$ be a set of polynomials, where $P_n(x)$ is of degree exactly n. Let α be a distribution function. If

$$\int_{-\infty}^{\infty} P_i(x)P_j(x)d\alpha(x) = \delta(i,j)\gamma_j \quad \text{(all } i,j\text{)},$$

where $\gamma_j \neq 0$ $(j\geq 0)$ and $\delta(i,j) = \begin{Bmatrix} 0, & i\neq j \\ 1, & i=j \end{Bmatrix}$, it is said that the sequence $\{P_n(x)\}$ is *orthogonal with respect to the distribution $d\alpha(x)$*. If $\gamma_j = 1$ $(j\geq 0)$, the word "orthogonal" is replaced by "orthonormal."

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*Since all the generalized weight functions considered here have compact support, the testing-function space can be taken to be C^∞, the space of all infinitely differentiable functions on $(-\infty,\infty)$.

Definition 3.8. Let α be a distribution function such that the support of $d\alpha(x)$ is contained in the closed (but not necessarily bounded) interval $[a,b]$, and let $\{P_n(x)\}$ be a sequence of polynomials such that $P_n(x)$ is of degree exactly n. If

$$\int_a^b P_i(x)P_j(x)d\alpha(x) = \delta(i,j)\gamma_j \quad (\text{all } i,j),$$

where $\gamma_j \neq 0$ $(\gamma_j=1)$ for all j, then $\{P_n(x)\}$ is said to be *orthogonal (orthonormal) on* $[a,b]$ *with respect to* $d\alpha(x)$. Moreover, if $d\alpha(x)$ is given by the weight function w on $[a,b]$, one says that $\{P_n(x)\}$ is *orthogonal (orthonormal) on* $[a,b]$ *with respect to the weight function* w.

When the terminology of Definition 3.8 is used, $[a,b]$ is usually understood to be the *smallest* closed interval containing the support of $d\alpha(x)$.

Now suppose that $d\alpha(x)$ is the *only* normalized distribution with respect to which $\{P_n(x)\}$ is orthogonal. It follows from the proof of Theorem 5.2.1 in Atkinson [3] that the smallest closed interval, say $[a,b]$, containing the support of $d\alpha(x)$ is contained in any closed interval which contains all the zeros of all the polynomials $P_n(x)$ $(n\geq 1)$. On the other hand, it is well known [19] that if $\{P_n(x)\}$ is orthogonal on $[a,b]$ with respect to $d\alpha(x)$--which is the case here--all the zeros of $P_n(x)$ $(n\geq 1)$ are contained in $[a,b]$. These considerations motivate the next definition.

Definition 3.9. Let $\{P_n(x)\}$ be a sequence of polynomials orthogonal with respect to some distribution. The *true interval of orthogonality* is the smallest closed interval containing all the zeros of all the polynomials $P_n(x)$ $(n \geq 1)$.

The sequences of polynomials considered in this study arise from three-term recurrences typified by

$$\begin{aligned} &P_{-1}(x) = 0, \quad P_0(x) = 1, \\ &P_{n+1}(x) = (A_n x + B_n)P_n(x) - C_n P_{n-1}(x), \quad n \geq 0, \end{aligned} \tag{P}$$

where A_n, B_n, C_n $(n \geq 0)$ are real constants ($C_0 \overset{d}{=} 1$ for convenience) and $A_n \neq 0$ $(n \geq 0)$. Such a recurrence generates a sequence of polynomials $\{P_n(x)\}$ in which $P_n(x)$ $(n \geq 0)$ has degree exactly n. The following theorem [9,13] gives a necessary and sufficient condition for $\{P_n(x)\}$ to be orthogonal with respect to a distribution.

Theorem 3.10. Let $\{P_n(x)\}$ be generated by (P). Then there is a distribution function α such that $\{P_n(x)\}$ is orthogonal with respect to $d\alpha(x)$ if and only if

$$\frac{C_n}{A_n A_{n-1}} > 0, \quad n \geq 1. \tag{1}$$

The connection between orthogonal polynomials generated by recurrence (P) and certain initial-value problems, of which [IVP] is a special case, is explained by a result of A. G. Law [13].

Theorem 3.11. Consider the initial-value problem

$$A_0X_0''(t) = B_0X_0(t) - X_1(t)$$

$$A_nX_n''(t) = -C_nX_{n-1}(t) + B_nX_n(t) - X_{n+1}(t), \quad n\geq 1,$$

$$X_n(0) = X_n'(0) = 0, \quad n\neq r,$$

$$X_r(0) = d_r, \quad X_r'(0) = v_r,$$

where A_n, B_n, C_n $(n\geq 0)$ are real constants $(C_0 \overset{d}{=} 1)$, and $A_n \neq 0$ $(n\geq 0)$. Let $\{P_n(x)\}$ satisfy recurrence (P); let (1) hold; let α be a distribution function such that $d\alpha(x)$ is normalized and such that $\{P_n(x)\}$ is orthogonal with respect to $d\alpha(x)$; let

$$\zeta_j = \int_{-\infty}^{\infty} [P_j(x)]^2 \, d\alpha(x), \quad j\geq 0; \tag{2}$$

and let

$$F(x,t) = \begin{cases} \dfrac{1}{\zeta_r} P_r(x)\left[d_r\cosh(t\sqrt{-x}) + \dfrac{v_r}{\sqrt{-x}}\sinh(t\sqrt{-x})\right], & x<0, \\[2ex] \dfrac{1}{\zeta_r} P_r(x)\left[d_r\cos(t\sqrt{x}) + \dfrac{v_r}{\sqrt{x}}\sin(t\sqrt{x})\right], & x\geq 0, \end{cases}$$

for all $t \geq 0$. Then a solution of the initial-value problem is given by

$$X_n(t) = \int_{-\infty}^{\infty} P_n(x)F(x,t)d\alpha(x), \quad n\geq 0, \ t\geq 0. \tag{3}$$

A companion result [13, p.14] gives a formula by which ζ_j (Equation (2)) can be computed, for any j, from the associated recurrence coefficients.

Theorem 3.12. Let $\{P_n(x)\}$ be the sequence of polynomials generated by (P); let (1) hold; and let α be as in Theorem 3.11. Then

$$\zeta_j \stackrel{d}{=} \int_{-\infty}^{\infty} [P_j(x)]^2 d\alpha(x) = \frac{A_0}{A_j} C_0 C_1 \cdots C_j \tag{4}$$

for $j\geq 0$.

From Theorem 3.11 it is seen that in order to write an explicit solution of [IVP] it suffices to know a distribution function α which gives a normalized distribution for the sequence of orthogonal polynomials satisfying the appropriate recurrence. The recurrence associated with [IVP] by Theorem 3.11 is

$$P_{-1}(x) = 0, \quad P_0(x) = 1,$$

$$P_{n+1}(x) = \left[-\frac{\mu_n m}{\lambda_{n+1}k} x + \left(1 + \frac{\lambda_n}{\lambda_{n+1}}\right)\right] P_n(x) - \frac{\lambda_n}{\lambda_{n+1}} P_{n-1}(x), \quad 0\leq n\leq N-1,$$

$$P_{n+1}(x) = \left(-\frac{m}{k} x + 2\right) P_n(x) - P_{n-1}(x), \quad n\geq N,$$

where $\lambda_N \overset{d}{=} 1$. Clearly condition (1) is satisfied by the coefficients. If

$$\tilde{P}_n(x) \overset{d}{=} P_n\left(-\frac{2k}{m}(x-1)\right), \quad n\geq 0,$$

then $\{\tilde{P}_n(x)\}$ satisfies the recurrence

$$\tilde{P}_{-1}(x) = 0, \quad \tilde{P}_0(x) = 1,$$

$$\tilde{P}_{n+1}(x) = \left[2\frac{\mu_n}{\lambda_{n+1}}x + \left(1 + \frac{\lambda_n}{\lambda_{n+1}} - \frac{2\mu_n}{\lambda_{n+1}}\right)\right]\tilde{P}_n(x) - \frac{\lambda_n}{\lambda_{n+1}}\tilde{P}_{n-1}(x), \quad 0\leq n\leq N-1,$$

$$\tilde{P}_{n+1}(x) = 2x\tilde{P}_n(x) - \tilde{P}_{n-1}(x), \quad n\geq N,$$

where $\lambda_N \overset{d}{=} 1$. Suppose that $\tilde{\alpha}$ is a distribution function such that $\tilde{P}_n(x)$ is orthogonal with respect to $d\tilde{\alpha}(x)$. If

$$\alpha(x) \overset{d}{=} -\tilde{\alpha}\left(-\frac{m}{2k}x + 1\right),$$

then α is a distribution function, and $\{P_n(x)\}$ is orthogonal with respect to $d\alpha(x)$ [2, p.196]. Thus, if a distribution for $\{\tilde{P}_n(x)\}$ were found, it would be possible to solve [IVP] by Theorem 3.11.

Toward the end of achieving greater generality, the following recurrence, of which the above recurrence is a special case, is considered.

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_{n+1}(x) = (2a_n x+b_n)R_n(x) - c_n R_{n-1}(x), \quad 0 \le n \le N-1, \tag{R}$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad n \ge N,$$

where N is a fixed non-negative integer, and $a_n \neq 0$ $(0 \le n \le N-1)$. The following problem is posed.

Problem II. Under the assumption that (R) generates a sequence $\{R_n(x)\}$ of orthogonal polynomials,* construct a distribution function α_R such that $\{R_n(x)\}$ is orthogonal with respect to $d\alpha_R(x)$.

There is a considerable body of literature [3,4,6,12,18] dealing with the general problem of finding a distribution for a sequence of orthogonal polynomials, given the three-term recurrence which it satisfies. These methods usually rely on known results concerning related classical moment problems [1,17], and they fail to take advantage of the "almost uniform" nature of recurrence (R).

Jayne [10,11] and Martens [15] have recently developed different

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*By Theorem 3.10, this assumption is equivalent to requiring that

$$\frac{c_n}{a_n a_{n-1}} > 0, \quad n=1,2,\cdots,N-1,$$

and

$$a_{N-1} > 0.$$

methods of constructing distribution functions that may be successfully applied to particular kinds of polynomial sequences. Jayne gives necessary and sufficient conditions on the recurrence coefficients for the polynomials of the associated sequence to be solutions of a second-order, linear, homogeneous, ordinary differential equation with polynomial coefficients. For such polynomials he gives a straightforward way of finding the associated differential equation, from which a distribution (given by a weight function) can be easily deduced. Unfortunately, the polynomials generated by (R) are solutions of a second-order differential equation only for a very few special cases. Martens' technique leads to the problem of solving an infinite system of algebraic equations. His method and subsequent modifications which take advantage of the special nature of (R) motivated the approach used in the present study (see Chapter IV).

To conclude this chapter, a general result about orthogonal polynomials is given. This result proves to be useful in the development of the solution of Problem II.

Theorem 3.13. Let $\{P_n(x)\}$ be a sequence of polynomials which is orthogonal with respect to some distribution. Let $\{\Pi_n(x)\}$ be a sequence of polynomials such that $\Pi_n(x)$ $(n\geq 0)$ is of degree exactly n. Let α be a distribution function, and suppose that there is an integer $K > 0$ such that

$$\int_{-\infty}^{\infty} P_n(x)\Pi_\nu(x)d\alpha(x) = \delta(n,\nu)\gamma_n, \quad \nu\leq n,$$

holds for all $n \geq K$, where $\gamma_n \neq 0$ $(n \geq K)$. Then $\{P_n(x)\}$ is orthogonal with respect to $d\alpha(x)$.

<u>Proof</u>. It suffices to establish that

$$\int_{-\infty}^{\infty} P_n(x)P_j(x)d\alpha(x) = \delta(n,j)\Lambda_n, \quad 0 \leq j \leq n, \tag{5}$$

holds for all $n \geq 0$, where $\Lambda_n \neq 0$ $(n \geq 0)$. Since $\Pi_\nu(x)$ $(\nu \geq 0)$ has degree exactly ν,

$$P_j(x) = \sum_{\nu=0}^{j} r_{j\nu}\Pi_\nu(x), \quad j \geq 0,$$

where $r_{j\nu}$ $(j \geq 0,\ \nu \leq j)$ is uniquely determined and $r_{jj} \neq 0$ $(j \geq 0)$. Hence, for fixed n $(n \geq 0)$, the relations

$$\int_{-\infty}^{\infty} P_n(x)\Pi_\nu(x)d\alpha(x) = \delta(n,\nu)\Gamma_n, \quad 0 \leq \nu \leq n, \tag{6}$$

where $\Gamma_n \neq 0$, imply (5). Therefore, it suffices to establish (6) for all $n \geq 0$. By hypothesis, (6) holds (with $\Gamma_n = \gamma_n$) for all $n \geq K$. It remains to show (6) for $0 \leq n \leq K-1$. The orthogonality of $\{P_n(x)\}$ implies that the polynomials $P_n(x)$ satisfy a recurrence [19] of type (P); and from Theorem 3.10 it follows that $\frac{C_n}{A_nA_{n-1}} > 0$ $(n \geq 1)$. Hence, $C_n \neq 0$ $(n \geq 1)$. The equations in recurrence (P) can be written

$$P_{\ell-1}(x) = \left[\frac{A_\ell}{C_\ell}x + \frac{B_\ell}{C_\ell}\right]P_\ell(x) - \frac{1}{C_\ell}P_{\ell+1}(x), \quad \ell \geq 1. \tag{7}$$

From this equation with $\ell = K$,

$$\int_{-\infty}^{\infty} P_{K-1}(x)\Pi_\nu(x)d\alpha(x) = \frac{A_K}{C_K}\int_{-\infty}^{\infty} P_K(x)[x\Pi_\nu(x)]d\alpha(x)$$

$$+ \frac{B_K}{C_K}\int_{-\infty}^{\infty} P_K(x)\Pi_\nu(x)d\alpha(x)$$

$$- \frac{1}{C_K}\int_{-\infty}^{\infty} P_{K+1}(x)\Pi_\nu(x)d\alpha(x), \quad 0\le\nu\le K-1.$$

By hypothesis, the last two integrals are zero. Moreover, the first integral is zero unless $\nu = K - 1$, for if $\nu < K - 1$, the polynomial $x\Pi_\nu(x)$ is of degree less than K and has an expansion as a linear combination of the $\Pi_j(x)$ $(0\le j\le \nu+1<K)$. Hence

$$\int_{-\infty}^{\infty} P_{K-1}(x)\Pi_\nu(x)d\alpha(x) = \delta(K-1,\nu)\Gamma_{K-1}, \quad 0\le\nu\le K-1,$$

where $\Gamma_{K-1} \overset{d}{=} \dfrac{A_K r_{K,K}\Gamma_K}{C_K A_{K-1} r_{K-1,K-1}} \neq 0$. Thus (6) holds for $n = K - 1$. That (6) holds for $0 \le n \le K - 2$ now follows from (7) by induction on q, where (7) is written (with $\ell=K-q$)

$$P_{K-q-1}(x) = \left[\frac{A_{K-q}}{C_{K-q}}x + \frac{B_{K-q}}{C_{K-q}}\right]P_{K-q}(x) - \frac{1}{C_{K-q}}P_{K-q+1}(x), \quad 0\le q\le K-1.$$

This concludes the proof.

CHAPTER IV

CONSTRUCTION OF THE ASSOCIATED DISTRIBUTION

At this stage, the problem of solving the basic initial-value problem [IVP] for the finitely defective semi-infinite linear chain has been reduced to the problem of finding a distribution function α_R such that the sequence $\{R_n(x)\}$ of orthogonal polynomials generated by the recurrence

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_{n+1}(x) = (2a_n x+b_n)R_n(x) - c_n R_{n-1}(x), \quad 0 \le n \le N-1, \tag{R}$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad n \ge N,$$

is orthogonal with respect to $d\alpha_R(x)$. The purpose of this chapter is to describe and justify a procedure for constructing such a distribution function.

Motivation for the approach used to arrive at this procedure came from earlier work by W. F. Martens [15] who solved [IVP] for the semi-infinite chain without initial spring in which the first mass is an isotope (see Figure 5).

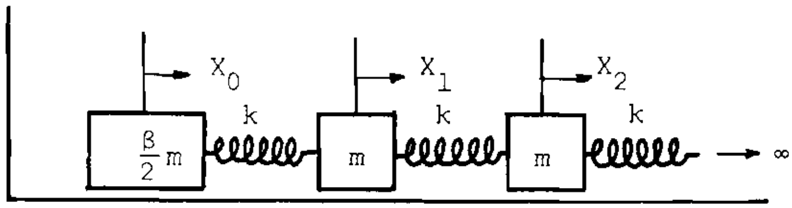


Figure 5. A Semi-Infinite Chain Considered by Martens

In order to apply Law's formula (Equation (3)), Martens produced a distribution for a sequence of polynomials satisfying a special case of (R). His results are summarized by the following.

(i) For a certain range of values of β the distribution has $[-1,1]$ as its support and is given by the weight function $\frac{w}{S}$, where w is the weight function for the sequence of Jacobi polynomials $\{P_n^{(-1/2,1/2)}(x)\}$ [19] and $S(x)$ is a first-degree polynomial whose coefficients are functions of β. The sequence $\{P_n^{(-1/2,1/2)}(x)\}$ is associated (after the change of variable described in Chapter III) with the uniform version of the chain in Figure 5 ($\beta=2$).

(ii) For the remaining values of β, the support of the distribution contains, in addition to $[-1,1]$, exactly one point x_1 outside $[-1,1]$. On $[-1,1]$, the distribution is again given by the weight function $\frac{w}{S}$. Thus, the distribution function can be described as the sum of an absolutely continuous function and a step function with a single point of increase at x_1 (the number x_1 is the limit of the sequence of smallest zeros of the associated sequence of polynomials).

It will be seen in the succeeding development that the results, even in the general case of (R), are strikingly similar to Martens'.

This chapter is organized into six sections:

Section 1. A Distribution for $\{R_n(x)\}$--Preliminary Definitions and Statement of the Result;

2. Representations of $R_n(x)$;

3. Properties of the Zeros of $P(z)$;

4. Verification of Orthogonality When $P(1) \neq 0$ and $P(-1) \neq 0$;

5. Verification of Orthogonality When $P(1) = 0$ or $P(-1) = 0$;

6. Normalization.

The main result of the chapter, Theorem 4.5, is given in section 1. This theorem and the definitions which precede it in order to make it statable give an outline of a procedure for constructing a distribution for $\{R_n(x)\}$. The proof of Theorem 4.5 is spread over sections 2-5. Sections 2 and 3 substantiate parts of the main theorem and contain information which is useful in applying the theorem to the solution of [IVP] (see Chapters V and VI). Sections 4 and 5 are concerned with the most important aspect of the proof: verification of the orthogonality of $\{R_n(x)\}$ with respect to the proposed distribution. Section 6 deals with normalization--i.e., the problem of obtaining a normalized distribution from the distribution given by Theorem 4.5.

A Distribution for $R_n(x)$ --Preliminary Definitions and Statement of the Result

Let $\{Q_n(x)\}$ be the sequence of polynomials generated by the recurrence

$$Q_{-1}(x) = 0, \quad Q_0(x) = 1,$$

$$Q_{n+1}(x) = 2xQ_n(x) - Q_{n-1}(x), \quad n\geq 0. \tag{Q}$$

The recurrence (Q) is (R) with $N = 0$, and $\{Q_n(x)\}$ is the sequence (after the change of variable discussed in Chapter III) of polynomials associated with a *uniform* semi-infinite chain of springs and masses (see Figure 1(a)). The polynomials $Q_n(x)$ $(n\geq 0)$ are the Chebyshev polynomials of the second kind [19]; $Q_n(x)$ is represented on $[-1,1]$ by

$$Q_n(x) = \frac{\sin(n+1)\theta}{\sin\theta}, \quad x=\cos\theta,\ n\geq 0; \tag{8}$$

and $\{Q_n(x)\}$ is orthonormal on $[-1,1]$ with respect to the weight function

$$w_Q(x) = \frac{2}{\pi}(1-x^2)^{1/2}, \quad -1\leq x\leq 1. \tag{9}$$

For each $n \geq 0$, $R_n(x)$ can be expressed as a real linear combination of $\{Q_\ell(x)\colon 0\leq \ell\leq n\}$. In particular, let

$$R_{2N}(x) = \beta_0 Q_{2N}(x) + \beta_1 Q_{2N-1}(x) + \cdots + \beta_{2N} Q_0(x). \tag{10}$$

The coefficients in this expression are used in the following definition.

<u>Definition 4.1</u>. Let β_ℓ $(0\leq\ell\leq 2N)$ be defined by (10). Then

$$P(z) \stackrel{d}{=} \sum_{\ell=0}^{2N} \beta_\ell z^\ell, \quad z \text{ complex}. \tag{11}$$

Since β_0 is the coefficient of $Q_{2N}(x)$ in (10), $P(0) = \beta_0 \neq 0$ ($P(z)$ may not have degree *exactly* $2N$, since it cannot be guaranteed in general that $\beta_\ell \neq 0$ if $\ell \neq 0$).

It can be shown that the product $P(e^{i\theta})P(e^{-i\theta})$, θ real, can be written uniquely as a real linear combination of $\cos q\theta$ $(0 \le q \le 2N)$. In turn, for each q $(0 \le q \le 2N)$, $\cos q\theta$ can be written uniquely as a real linear combination of $\cos^j \theta$ $(0 \le j \le q)$. Thus, there is a unique set of real constants $\alpha_0, \alpha_1, \cdots, \alpha_{2N}$ such that

$$P(e^{i\theta})P(e^{-i\theta}) = \sum_{\ell=0}^{2N} \alpha_\ell \cos^\ell \theta. \tag{12}$$

The coefficients in this expression are used as follows.

<u>Definition 4.2</u>. Let α_ℓ $(0 \le \ell \le 2N)$ be defined by (12). Then

$$S(z) \overset{d}{=} \sum_{\ell=0}^{2N} \alpha_\ell z^\ell, \quad z \text{ complex}.$$

Since the coefficients $\beta_0, \cdots, \beta_{2N}$ are real, $P(e^{-i\theta}) = \overline{P(e^{i\theta})}$; hence, from (12) the following representation of $S(x)$ for $-1 \le x \le 1$ is obtained:

$$S(x) = |P(e^{i\theta})|^2, \quad x = \cos\theta. \tag{13}$$

Consequently $S(x) \ge 0$ on $[-1,1]$, and $S(x_0) = 0$ for some $x_0 \varepsilon [-1,1]$ if and only if $P(e^{i\theta_0}) = 0$, where $x_0 = \cos\theta_0$. Thus, the zeros of $S(x)$ in

$[-1,1]$ correspond to zeros of $P(z)$ on the unit circle $|z| = 1$.

Two functions which are used to construct a distribution for $\{R_n(x)\}$ are now defined.

Definition 4.3. Let w_Q be given by (9) and let the polynomial $S(x)$ be given by Definition 4.2. Suppose that

$$\int_{-1}^{1} \frac{w_Q(y)}{S(y)}\, dy \tag{14}$$

exists. Then

$$\alpha_1(x) \overset{d}{=} \int_{-1}^{x} \frac{w_Q(y)}{S(y)}\, dy, \quad -1\le x\le 1; \tag{15}$$

also, $\alpha_1(x) \overset{d}{=} \alpha_1(-1) = 0$ on $(-\infty,-1)$, and $\alpha_1(x) \overset{d}{=} \alpha_1(1)$ on $(1,\infty)$.

Definition 4.4. Let the polynomial $P(z)$ be defined by (11). If $P(z)$ has p $(p>0)$ zeros in the real interval $(-1,1)$ and if each of these zeros is simple, let them be labeled $z_1, z_2, \cdots, z_p$ in such a manner that the numbers $x_1, x_2, \cdots, x_p$ given by

$$x_j = \frac{1}{2}\,(z_j + z_j^{-1}), \quad 1\le j\le p,$$

obey $x_1 < x_2 < \cdots < x_p$. Suppose that $P(z_j^{-1}) \neq 0$ $(1\le j\le p)$. Then

$$\alpha_2(x) \overset{d}{=} \begin{cases} 0, & -\infty<x<x_1, \\ \displaystyle\sum_{j=1}^{\ell} \frac{(z_j-z_j^{-1})^2}{z_j P'(z_j)P(z_j^{-1})}, & x_\ell \le x < x_{\ell+1}, \\ & \ell=1,2,\cdots,p-1, \\ \displaystyle\sum_{j=1}^{p} \frac{(z_j-z_j^{-1})^2}{z_j P'(z_j)P(z_j^{-1})}, & x \ge x_p \end{cases} \tag{16}$$

(recall that $P(0) \neq 0$ by the remarks following Definition 4.1). If $P(z)$ has no zeros in $(-1,1)$,

$$\alpha_2(x) \overset{d}{=} 0. \tag{17}$$

The following result asserts that the definitions of α_1 and α_2 are always meaningful and that $\alpha_1 + \alpha_2$ is a distribution function for $\{R_n(x)\}$.

<u>Theorem 4.5</u>. Let $\{R_n(x)\}$ be generated by (R), and let $P(z)$ be defined by (11). Then

(i) the integral (14) exists;

(ii) the zeros of $P(z)$ in the real interval $(-1,1)$ are simple, and $P(\hat{z}^{-1}) \neq 0$ whenever $\hat{z}$ is a zero of $P(z)$ in $(-1,1)$;

(iii) $\alpha_R \overset{d}{=} \alpha_1 + \alpha_2$ is a distribution function; and

(iv) $\{R_n(x)\}$ is orthogonal with respect to $d\alpha_R(x)$.

The conclusion of Theorem 4.5 can be summarized as follows.

(i) If $P(z)$ has no zeros in $(-1,1)$, there is an absolutely continuous distribution function α_R ($\alpha_R = \alpha_1$) for $\{R_n(x)\}$. The support of the distribution $d\alpha_R(x)$ is the interval $[-1,1]$ and $d\alpha_R(x)$ is given by the weight function $\frac{w_Q(x)}{S(x)}$, where w_Q is the weight function for $\{Q_n(x)\}$ and $S(x)$ is a polynomial of degree at most $2N$.

(ii) If $P(z)$ has zeros $z_1,\cdots,z_p$ in $(-1,1)$, the distribution function α_R for $\{R_n(x)\}$ is the sum of an absolutely continuous function α_1 on $[-1,1]$ and a step function α_2 with jumps $J(x_j)$ at $x_j \overset{d}{=} \frac{1}{2}(z_j+z_j^{-1})$ $(1\le j\le p)$, where

$$J(x_j) = \frac{(z_j-z_j^{-1})^2}{z_j P'(z_j)P(z_j^{-1})} .$$

The numbers x_j $(1\le j\le p)$ are outside $[-1,1]$. Thus the support of $d\alpha_R(x)$ is $[-1,1] \cup \{x_j\colon 1\le j\le p\}$ and a (generalized) weight function is

$$w(x) = \frac{w_Q(x)}{S(x)} H(1+x)H(1-x) + \sum_{j=1}^{p} J(x_j)\delta(x-x_j),$$

where H is the Heaviside unit step function and δ is the Dirac delta function.

As a corollary to Theorem 4.5, a statement may be made about the true interval of orthogonality.

<u>Corollary 4.6</u>. If $P(z)$ has zeros $z_1,\cdots,z_p$ in $(-1,1)$, let them be labeled as in Definition 4.4, and let $x_j = \frac{1}{2}(z_j+z_j^{-1})$ $(1\le j\le p)$. Let

$$a = \begin{cases} -1, & \text{if } P(z) \text{ has no zeros in } (-1,1), \\ \min\{x_1,-1\}, & \text{otherwise;} \end{cases}$$

$$b = \begin{cases} 1, & \text{if } P(z) \text{ has no zeros in } (-1,1), \\ \max\{x_p,1\}, & \text{otherwise.} \end{cases}$$

Then $[a,b]$ is the true interval of orthogonality for $\{R_n(x)\}$.

As mentioned in the introduction to this chapter, the proof of Theorem 4.5 is spread over the next four sections. The proof involves two things:

(i) showing that the definitions of α_1 and α_2 are always meaningful and that $\alpha_1 + \alpha_2$ is a distribution function; and

(ii) verifying the orthogonality of $\{R_n(x)\}$ with respect to $d\alpha_R(x)$.

Item (i) constitutes the results of section 3, which are established by using a representation for $\{R_n(x)\}$ deduced in section 2. Item (ii) is accomplished in sections 4 and 5--the verification of orthogonality requiring results from section 3 and an additional representation from section 2.

Finally, it should be observed that S. Bernstein [5] considered weight functions on $[-1,1]$ of the form $\frac{w_Q}{\rho}$, where $\rho(x)$ is a polynomial and $\rho(x) > 0$ on $[-1,1]$. He found that the associated orthogonal polynomials have the properties exhibited in this study by $\{R_n(x)\}$ when $P(z)$ has no zeros in the closed interval $[-1,1]$. One of Bernstein's results is mentioned in section 2.

Representations of $R_n(x)$

The purpose of this section is to present two important representations of $R_n(x)$. The first one is the trigonometric representation given by Theorem 4.9 (Equation (25)). It is used in the verification of orthogonality (sections 4 and 5). The second representation is given by Theorem 4.11 (Equation (27)). It is used in verifying some of the properties of the zeros of $P(z)$ (section 3). These representations are also useful when applying the results of this chapter to the solution of [IVP]. In addition (24) should be mentioned as a means of finding the coefficients of $P(z)$ (it is not used, however, in the applications discussed in this study).

Lemma 4.7. For every complex number x,

$$R_n(x) = Q_{n-N}(x)R_N(x) - Q_{n-N-1}(x)R_{N-1}(x), \quad n\geq N. \tag{18}$$

Proof. If $n = N$, the assertion follows immediately from recurrence (Q). Let $j > N$, and suppose that (18) holds for all n satisfying $N \leq n \leq j$. This assumption and recurrences (R) and (Q) yield

$$R_{j+1}(x) = 2xR_j(x) - R_{j-1}(x)$$

$$= 2x[Q_{j-N}(x)R_N(x)-Q_{j-N-1}(x)R_{N-1}(x)]$$

$$- [Q_{j-1-N}(x)R_N(x)-Q_{j-2-N}(x)R_{N-1}(x)]$$

$$= [2xQ_{j-N}(x)-Q_{j-N-1}(x)]R_N(x)$$

$$- [2xQ_{j-N-1}(x)-Q_{j-N-2}(x)]R_{N-1}(x)$$

$$= Q_{(j+1)-N}(x)R_N(x) - Q_{(j+1)-N-1}R_{N-1}(x).$$

By induction (18) is established for all $n \geq N$.

Lemma 4.8. Let the real constants $\beta_0,\cdots,\beta_{2N}$ be defined by Equation (10). Then, for every complex number x,

$$R_n(x) = \sum_{\ell=0}^{2N} \beta_\ell Q_{n-\ell}(x), \quad n\geq 2N. \tag{19}$$

Proof. Equation (19) holds for n = 2N by definition of β_ℓ $(0\leq\ell\leq 2N)$; so (19) must be substantiated for n > 2N. It suffices to verify (19) for n = 2N + 1; for once this fact is established, the hypothesis that (19) holds for all n such that $2N + 1 \leq n \leq j$ $(j>2N+1)$ can be combined with recurrences (R) and (Q) to yield

$$R_{j+1}(x) = 2xR_j(x) - R_{j-1}(x)$$

$$= 2x \sum_{\ell=0}^{2N} \beta_\ell Q_{j-\ell}(x) - \sum_{\ell=0}^{2N} \beta_\ell Q_{j-1-\ell}(x)$$

$$= \sum_{\ell=0}^{2N} \beta_\ell [2xQ_{j-\ell}(x) - Q_{j-\ell-1}(x)]$$

$$= \sum_{\ell=0}^{2N} \beta_\ell Q_{(j+1)-\ell}(x),$$

thereby proving (19) inductively for all $n \geq 2N + 1$.

Accordingly, let γ_ℓ $(0 \leq \ell \leq 2N+1)$ be defined by

$$R_{2N+1}(x) = \sum_{\ell=0}^{2N+1} \gamma_\ell Q_{2N+1-\ell}(x).$$

It will be shown that $\gamma_{2N+1} = 0$ and that $\gamma_\ell = \beta_\ell$ for $0 \leq \ell \leq 2N$, results which establish (19) for $n = 2N + 1$.

The sequence $\{Q_n(x)\}$ is orthonormal on $[-1,1]$ with respect to the weight function w_Q; this fact and identity (18) (with $n=2N+1$) imply that

$$\gamma_{2N+1} = \int_{-1}^{1} R_{2N+1}(x)Q_0(x)w_Q(x)dx$$

$$= \int_{-1}^{1} R_{2N+1}(x)w_Q(x)dx$$

$$= \int_{-1}^{1} Q_{N+1}(x)R_N(x)w_Q(x)dx - \int_{-1}^{1} Q_N(x)R_{N-1}(x)w_Q(x)dx.$$

But $Q_\nu(x)$ is orthogonal to every polynomial of degree less than ν.

Hence, $\gamma_{2N+1} = 0$.

Now it is shown that $\gamma_\ell = \beta_\ell$ $(0 \le \ell \le 2N)$ by computing each of these sets of coefficients and comparing the results. Let

$$R_{N-1}(x) = \sum_{j=0}^{N-1} q_j Q_{N-j-1}(x), \tag{20}$$

and let

$$R_N(x) = \sum_{j=0}^{N} p_j Q_{N-j}(x). \tag{21}$$

Then, from (18) (with n=2N), (20), and (21),

$$\begin{aligned}
\beta_\ell &= \int_{-1}^{1} Q_{2N-\ell}(x) R_{2N}(x) w_Q(x)\,dx \\
&= \int_{-1}^{1} Q_{2N-\ell}(x)[Q_N(x)R_N(x) - Q_{N-1}(x)R_{N-1}(x)]w_Q(x)\,dx \\
&= \sum_{j=0}^{N} p_j \int_{-1}^{1} Q_{2N-\ell}(x)[Q_N(x)Q_{N-j}(x)]w_Q(x)\,dx \\
&\quad - \sum_{j=0}^{N-1} q_j \int_{-1}^{1} Q_{2N-\ell}(x)[Q_{N-1}(x)Q_{N-j-1}(x)]w_Q(x)\,dx, \quad 0 \le \ell \le 2N.
\end{aligned}$$

Now use the following identity, which can be verified by means of (Q) or the trigonometric representation (8):

$$Q_i(x)Q_j(x) = \sum_{\nu=0}^{i} Q_{j-i+2\nu}(x), \quad -1 \le i \le j \tag{22}$$

(the sum on the right side is taken to be zero if i = -1). This identity and the orthonormality of $Q_n(x)$ yield

$$\beta_\ell = \sum_{j=0}^{N} p_j \sum_{\nu=0}^{N-j} \int_{-1}^{1} Q_{2N-\ell}(x)Q_{j+2\nu}(x)w_Q(x)dx$$

$$- \sum_{j=0}^{N-1} q_j \sum_{\nu=0}^{N-j-1} \int_{-1}^{1} Q_{2N-\ell}(x)Q_{j+2\nu}(x)w_Q(x)dx$$

$$= \sum_{j=0}^{N} p_j \sum_{\nu=0}^{N-j} \delta(2N-\ell,j+2\nu) - \sum_{j=0}^{N-1} q_j \sum_{\nu=0}^{N-j-1} \delta(2N-\ell,j+2\nu). \qquad (23)$$

Similarly, for $0 \le \ell \le 2N$,

$$\gamma_\ell = \int_{-1}^{1} Q_{2N+1-\ell}(x)R_{2N+1}(x)w_Q(x)dx$$

$$= \sum_{j=0}^{N} p_j \int_{-1}^{1} Q_{2N+1-\ell}(x)[Q_{N+1}(x)Q_{N-j}(x)]w_Q(x)dx$$

$$- \sum_{j=0}^{N-1} q_j \int_{-1}^{1} Q_{2N+1-\ell}(x)[Q_N(x)Q_{N-j-1}(x)]w_Q(x)dx$$

$$= \sum_{j=0}^{N} p_j \sum_{\nu=0}^{N-j} \int_{-1}^{1} Q_{2N+1-\ell}(x)Q_{j+2\nu+1}(x)w_Q(x)dx$$

$$- \sum_{j=0}^{N-1} q_j \sum_{\nu=0}^{N-j-1} \int_{-1}^{1} Q_{2N+1-\ell}(x)Q_{j+2\nu+1}(x)w_Q(x)dx$$

$$= \sum_{j=0}^{N} p_j \sum_{\nu=0}^{N-j} \delta(2N+1-\ell,j+2\nu+1)$$

$$- \sum_{j=0}^{N-1} q_j \sum_{\nu=0}^{N-j-1} \delta(2N+1-\ell, j+2\nu+1).$$

Comparison of the last result with (23) shows that $\gamma_\ell = \beta_\ell$ for $0 \leq \ell \leq 2N$. Thus (19) is verified for $n = 2N + 1$. By remarks made earlier, this concludes the proof.

The procedure described for constructing a distribution for $\{R_n(x)\}$ depends heavily on the polynomial $P(z)$ with coefficients β_ℓ $(0 \leq \ell \leq 2N)$. Note that these coefficients can be computed by using Equation (23), provided the coefficients p_j $(0 \leq j \leq N)$ and q_j $(0 \leq j \leq N-1)$ in the representations of $R_N(x)$ and $R_{N-1}(x)$ as linear combinations of the $Q_n(x)$ are known. For the particular linear chains considered in the present study (Chapters V and VI), the p_j's and q_j's are obtained fairly easily from the recurrence. Rather than using (23), however, it seems less difficult in the particular cases considered to use (18) and (22) to obtain representation (19) for $R_{2N}(x)$, from which the β_ℓ's can be read directly. Nevertheless, the following reduction of (23) can be established and is recorded for possible future usefulness.

$$\beta_0 = p_0,$$

$$\beta_1 = p_1, \tag{24}$$

$$\beta_\ell = \sum_{\substack{0 \leq j \leq n_1 \\ (j \text{ even})}} p_j - \sum_{\substack{0 \leq j \leq n_2 \\ (j \text{ even})}} q_j, \quad \ell \text{ even}, \ \ell \geq 2,$$

$$\beta_\ell = \sum_{\substack{0\le j\le n_1\\(j\text{ odd})}} p_j - \sum_{\substack{0\le j\le n_2\\(j\text{ odd})}} q_j,\ \ell\text{ odd},\ \ell\ge 3,$$

where $n_1 = \min\{\ell, 2N-\ell\}$, and $n_2 = \min\{\ell-2, 2N-\ell\}$.

Lemma 4.8 leads now to one of the trigonometric representations desired for $R_n(x)$ $(n\ge N-1)$ on $[-1,1]$. Under more restrictive conditions, this representation was known to Bernstein [19, p.31].

<u>Theorem 4.9</u>. Let $P(z)$ be given by Definition 4.1. Then, for all $n \ge N - 1$,

$$R_n(x) = \frac{1}{\sin\theta}\,\mathit{Im}\{e^{i(n+1)\theta}P(e^{-i\theta})\},\quad x=\cos\theta. \tag{25}$$

<u>Proof</u>. For $n \ge 2N$, Equations (19) (with $x=\cos\theta$), (8), and (11) yield

$$\begin{aligned} R_n(\cos\theta) &= \sum_{\ell=0}^{2N} \beta_\ell Q_{n-\ell}(\cos\theta) \\ &= \sum_{\ell=0}^{2N} \beta_\ell \frac{\sin(n-\ell+1)\theta}{\sin\theta} \\ &= \frac{1}{\sin\theta}\,\mathit{Im}\left\{\sum_{\ell=0}^{2N} \beta_\ell e^{i(n-\ell+1)\theta}\right\} \\ &= \frac{1}{\sin\theta}\,\mathit{Im}\left\{e^{i(n+1)\theta}\sum_{\ell=0}^{2N}\beta_\ell e^{-i\ell\theta}\right\} \\ &= \frac{1}{\sin\theta}\,\mathit{Im}\left\{e^{i(n+1)\theta}P(e^{-i\theta})\right\}. \end{aligned}$$

Thus (25) is verified for $n \geq 2N$. The situation when $N - 1 \leq n < 2N$ is now examined. The equations in (R) can be written (with $x=\cos\theta$)

$$R_{2N-j}(\cos\theta) = (2\cos\theta)R_{2N-j+1}(\cos\theta) - R_{2N-j+2}(\cos\theta), \quad 1\leq j\leq N+1, \quad (26)$$

which gives R_n in terms of R_{n+1} and R_{n+2} for $N - 1 \leq n \leq 2N - 1$. Now (25) with $n = 2N$ and $n = 2N + 1$, together with (26) (with $j=1$), yields

$$\begin{aligned}
R_{2N-1}(\cos\theta) &= (2\cos\theta)R_{2N}(\cos\theta) - R_{2N+1}(\cos\theta) \\
&= (2\cos\theta)\frac{1}{\sin\theta}\, Im\,\{e^{i(2N+1)\theta}P(e^{-i\theta})\} \\
&\quad - \frac{1}{\sin\theta}\, Im\,\{e^{i(2N+2)\theta}P(e^{-i\theta})\} \\
&= \frac{1}{\sin\theta}\, Im\{[2e^{i(2N+1)\theta}\cos\theta - e^{i(2N+2)\theta}]P(e^{-i\theta})\} \\
&= \frac{1}{\sin\theta}\, Im\,\{e^{i(2N)\theta}P(e^{-i\theta})\}.
\end{aligned}$$

Thus (25) is established for $n = 2N - 1$. An induction on j using (26) verifies (25) for $N - 1 \leq n \leq 2N - 2$. This concludes the proof.

It proves necessary also to examine $R_n(x)$ for x in the complex plane outside $[-1,1]$. For this purpose, the following mapping is introduced.

<u>Definition 4.10</u>. For $0 < |z| < 1$, let $H(z) = \dfrac{z + z^{-1}}{2}$.

Then H is a one-to-one analytic mapping of the interior of the punctured unit disk onto the exterior of the closed real interval $[-1,1]$. Moreover, H maps the real interval $(-1,0)$ onto the real interval $(-\infty,-1)$ and the real interval $(0,1)$ onto the real interval $(1,\infty)$. The representation theorem is now stated.

<u>Theorem 4.11</u>. For $0 < |z| < 1$,

$$R_n(H(z)) = \frac{z^{n+1}P(z^{-1}) - z^{-(n+1)}P(z)}{z - z^{-1}}, \quad n\geq 2N. \tag{27}$$

<u>Proof</u>. Since Equation (19) is used to establish the result, a representation of $Q_n\left(\frac{z+z^{-1}}{2}\right)$ is needed. To this end, first let $z = e^{i\theta}$. Then by (8),

$$Q_n\left(\frac{z+z^{-1}}{2}\right) = Q_n\left(\frac{e^{i\theta}+e^{-i\theta}}{2}\right)$$

$$= Q_n(\cos\theta)$$

$$= \frac{\sin(n+1)\theta}{\sin\theta}$$

$$= \frac{e^{i(n+1)\theta} - e^{-i(n+1)\theta}}{e^{i\theta} - e^{-i\theta}},$$

or

$$Q_n\left(\frac{z+z^{-1}}{2}\right) = \frac{z^{n+1} - z^{-(n+1)}}{z - z^{-1}}, \tag{28}$$

for $|z| = 1$, and $n \geq 0$. For all $z \neq 0$, the left and right sides of (28) define two analytic functions. Since (by (28)) these functions agree for $|z| = 1$, they are equal for all $z \neq 0$. Combining (19), the representation (28), and the definition of $P(z)$ now yields

$$\begin{aligned}
R_n\left(\frac{z+z^{-1}}{2}\right) &= \sum_{\ell=0}^{2N} \beta_\ell Q_{n-\ell}\left(\frac{z+z^{-1}}{2}\right) \\
&= \sum_{\ell=0}^{2N} \beta_\ell \frac{z^{n-\ell+1} - z^{-(n-\ell+1)}}{z - z^{-1}} \\
&= \frac{1}{z - z^{-1}}\left[z^{n+1}\sum_{\ell=0}^{2N} \beta_\ell z^{-\ell} - z^{-(n+1)}\sum_{\ell=0}^{2N} \beta_\ell z^{\ell}\right] \\
&= \frac{z^{n+1}P(z^{-1}) - z^{-(n+1)}P(z)}{z - z^{-1}}, \quad n \geq 2N,\ z \neq 0.
\end{aligned} \tag{29}$$

The restriction $0 < |z| < 1$ gives (27). This concludes the proof.

Properties of the Zeros of $P(z)$

This section is concerned with the location and multiplicity of the zeros of $P(z)$. To indicate why the results obtained are needed, their part in the proof of Theorem 4.5 is first described.

(i) By Lemma 4.20, $\int_{-1}^{1} \frac{w_Q(x)}{S(x)}\,dx$ ((14)) exists. This result is conclusion (i) of Theorem 4.5.

(ii) By Lemma 4.14, the zeros of $P(z)$ in $(-1,1)$ are simple, and by Lemma 4.16, $P(\hat{z}^{-1}) \neq 0$ whenever $\hat{z}$ is a zero of $P(z)$ in $(-1,1)$. This is conclusion (ii) of Theorem 4.5.

(iii) By (i), it is possible to define α_1 by Equation (15). Moreover, by Lemma 4.20, $\frac{w_Q(x)}{S(x)} > 0$ on $(-1,1)$; so α_1 is a *distribution function*. If $P(z)$ has zeros $z_1, \cdots, z_p$ in $(-1,1)$ (as in Definition 4.4), item (ii) guarantees that α_2 can be defined by (16). In addition, Lemma 4.17 shows that the jumps in the step function α_2 are nonnegative (in fact, positive). Thus, α_2 is non-decreasing--a result which also holds trivially if $P(z)$ does not have zeros in $(-1,1)$, since in that case, $\alpha_2(x) \equiv 0$. Now let $\alpha_R = \alpha_1 + \alpha_2$. Since α_1 is a distribution function and α_2 is nondecreasing and bounded, it follows that α_R is a distribution function. This is conclusion (iii) of Theorem 4.5.

(iv) It remains to verify the orthogonality of $\{R_n(x)\}$ with respect to $d\alpha_R(x)$, which is done in sections 4 and 5. There the integral involved is transformed into a contour integral around the unit circle $|z| = 1$, and the zeros of $P(z)$ in $|z| \leq 1$ turn out to be singularities of the integrand. The results of the present section which are subsequently used in the orthogonality proof are that the zeros of $P(z)$ in $|z| < 1$ (if there are any) are real (Corollary 4.13) and simple (Lemma 4.14), that the zeros of $P(z)$ on $|z| = 1$ (if there are any) are 1 and -1 (Lemma 4.18), and that if 1 or -1 is a zero of $P(z)$, it is simple (Lemma 4.19).

Theorem 4.11 and the orthogonality of $\{R_n(x)\}$ (as assumed a priori) are helpful in establishing properties of the zeros of $P(z)$ in this section. Generally speaking, the location and multiplicity of the zeros of $P(z)$ are related via (27) to the properties of the zeros of $\{R_n(x)\}$.

In the succeeding development, let Z denote the set consisting of all the zeros of all the polynomials $R_n(x)$ $(n \geq 1)$; i.e., let

$$Z = \{z\colon \ R_n(z) = 0 \ \text{ for some } n \geq 1\}.$$

Let

$$\Delta_1 = \{z\colon \ |z| < 1\}.$$

The first lemma establishes a one-to-one correspondence, by way of the mapping H (Definition 4.10), between the limit points of Z outside $[-1,1]$ and the zeros of $P(z)$ in Δ_1. It follows from this result that $P(z)$ can have only real zeros in Δ_1.

<u>Lemma 4.12</u>. Let $\hat{x}$ be a complex number, $\hat{x} \notin [-1,1]$. Then $\hat{x}$ is a limit point of Z if and only if $P(H^{-1}(\hat{x})) = 0$.

<u>Proof</u>. Suppose $P(\hat{z}) = 0$, where $\hat{z} \overset{d}{=} H^{-1}(\hat{x})$. Let W be any open disk centered at $\hat{x}$ and such that $W \cap [-1,1] = \emptyset$. It is now shown that $W - \{\hat{x}\}$ contains an element of Z. $H^{-1}[W]$ is an open subset of the open set $\Delta_1 - \{0\}$. Moreover, $\hat{z} \in H^{-1}[W]$, and the zeros of $P(z)$ are isolated. Consequently, there exists a closed disk D, centered at $\hat{z}$, with the following properties:

(i) $0 \notin D$;

(ii) $D \subset H^{-1}[W] \subset \Delta_1$;

(iii) $P(z) \neq 0$ for $z \in \partial D$.

Let such a disk be chosen, say $D = \{z: |z-\hat{z}| \leq \delta\}$. Let

$$m = \min_{z \in \partial D} |P(z)|$$

and

$$M = \max_{z \in \partial D} |P(z^{-1})|.$$

The continuity of P on ∂D guarantees the existence of m, and by (iii) $m > 0$. Also, by (i) and the continuity of the mapping $u = P(z^{-1})$, the existence of M is ensured. Thus, for $z \in \partial D$ and $n \geq 0$,

$$|z^{n+1} P(z^{-1})| \leq |z|^{n+1} M \leq (|\hat{z}|+\delta)^{n+1} M < M \tag{30}$$

and

$$|z^{-(n+1)} P(z)| \geq |z|^{-(n+1)} m \geq (|\hat{z}|+\delta)^{-(n+1)} m. \tag{31}$$

Since $|\hat{z}| + \delta < 1$ (by (ii)), there is an integer N_0, which can be taken to be greater than 2N, such that

$$(|\hat{z}|+\delta)^{-(N_0+1)} > \frac{M}{m}.$$

This inequality and (30) and (31) (with $n=N_0$) yield

$$\left|z^{-(N_0+1)}P(z)\right| \geq (|\hat{z}|+\delta)^{-(N_0+1)}m > \frac{M}{m}\cdot m = M > \left|z^{N_0+1}P(z^{-1})\right|$$

for all $z \in \partial D$. Hence, by Rouché's Theorem, the functions G and K, analytic on D and defined there by

$$G(z) = z^{N_0+1}P(z^{-1}) - z^{-(N_0+1)}P(z)$$

and

$$K(z) = z^{-(N_0+1)}P(z),$$

have the same number of zeros in the interior of D. But $\hat{z} \in \text{int}(D)$ and by hypothesis $P(\hat{z}) = 0$. So $K(z)$ has at least one zero in the interior of D. Therefore, there exists $z_1 \in \text{int}(D)$ such that $G(z_1) = 0$. Now by (27)

$$R_{N_0}\left(H(z_1)\right) = \frac{G(z_1)}{z_1 - z_1^{-1}} = 0.$$

Let $x_1 = H(z_1)$. Then $R_{N_0}(x_1) = 0$. Hence $x_1 \in Z$. Moreover, $x_1 \in H[D]$ and $H[D] \subset W$; therefore, $x_1 \in W$. It must be shown, however, that $x_1 \neq \hat{x}$. Suppose, to the contrary, that $x_1 = \hat{x}$. Then $z_1 = \hat{z}$, since H is one-to-one. But $z_1 = \hat{z}$ implies that

$$0 = G(z_1) = G(\hat{z}) = \hat{z}^{N_0+1}P(\hat{z}^{-1}) - \hat{z}^{-(N_0+1)}P(\hat{z}).$$

But $P(\hat{z}) = 0$; so

$$\hat{z}^{N_0+1} P(\hat{z}^{-1}) = 0.$$

Since $\hat{z} \neq 0$, $P(\hat{z}^{-1}) = 0$. Hence, for each $n \geq 2N$,

$$R_n(\hat{x}) = R_n\big(H(\hat{z})\big) = \frac{\hat{z}^{n+1}P(\hat{z}^{-1}) - \hat{z}^{-(n+1)}\, P(\hat{z})}{\hat{z} - \hat{z}^{-1}} = 0.$$

However, this equation cannot hold for *all* $n \geq 2N$ because of the interlacing property of the zeros of the polynomials $R_n(x)$ $(n \geq 1)$. Since the supposition that $x_1 = \hat{x}$ leads to a contradiction, it must be the case that $x_1 \neq \hat{x}$. Hence $x_1 \in Z \cap (W - \{\hat{x}\})$, which concludes the proof of sufficiency.

Now suppose that $\hat{x}$ is a limit point of Z; and suppose, contrary to the assertion of the lemma, that $P(\hat{z}) \neq 0$, where $\hat{z} \stackrel{d}{=} H^{-1}(\hat{x})$. Then there exists a disk $D_1 = \{z\colon |z-\hat{z}| \leq \delta_1\}$ such that $D_1 \subset \Delta_1 - \{0\}$ and $P(z) \neq 0$ for all $z \in D_1$. If

$$m_1 = \min_{z \in \partial D_1} |P(z)|$$

and

$$M_1 = \max_{z \in \partial D_1} |P(z^{-1})|,$$

then $m_1 > 0$. As in the proof of sufficiency, the inequalities

$$|z^{n+1}\,P(z^{-1})| < M_1$$

and

$$|z^{-(n+1)}\,P(z)| \geq (|\hat{z}|+\delta_1)^{-(n+1)}\,m_1$$

hold for all $z \in \partial D_1$ and for all $n \geq 0$. Since $|\hat{z}| + \delta_1 < 1$, there is an integer $N_1 \geq 2N$ such that

$$(|\hat{z}|+\delta_1)^{-(n+1)} > \frac{M_1}{m_1}$$

for all $n \geq N_1$. Therefore

$$|z^{-(n+1)}\,P(z)| > |z^{n+1}\,P(z^{-1})|$$

for all $z \in \partial D_1$ and all $n \geq N_1$. By Rouché's Theorem, it follows that for each $n \geq N_1$ the functions G_n and K_n defined by

$$G_n(z) = z^{n+1}\,P(z^{-1}) - z^{-(n+1)}\,P(z)$$

and

$$K_n(z) = z^{-(n+1)}\,P(z)$$

have the same number of zeros in the interior of D_1. But $K_n(z) \neq 0$ for all $z \in D_1$, by the way in which D_1 was chosen. Therefore, $G_n(z)$ has no zeros in the interior of D_1. This implies, by way of (27), that

$$R_n\big(H(z)\big) \neq 0, \quad n \geq N_1, \quad z \in \mathrm{int}(D_1). \tag{32}$$

Let $W_1 = H[\mathrm{int}(D_1)]$. By the analyticity of H, W_1 is an open set; moreover $\hat{x} \in W_1$. But, if $x \in W_1$, then $x = H(z)$ for some $z \in \mathrm{int}(D_1)$, and by (32), $R_n(x) \neq 0$ for all $n \geq N_1$. Hence W_1 is a neighborhood of $\hat{x}$ which contains only finitely many elements of Z (at most the zeros of $R_n(x)$ for $1 \leq n < N_1$). This contradicts the hypothesis that $\hat{x}$ is a limit point of Z. It follows that the assumption $P(\hat{z}) \neq 0$ is false. Thus $P(\hat{z}) = 0$. This completes the proof.

Corollary 4.13. If $|\hat{z}| < 1$ and $P(\hat{z}) = 0$, then $\hat{z}$ is real.

Proof. Let $|\hat{z}| < 1$ and $P(\hat{z}) = 0$. Then $\hat{z} \neq 0$ (see remarks following Definition 4.1). Let $\hat{x} = H(\hat{z})$. By Lemma 4.12, $\hat{x}$ is a limit point of Z. But all the zeros of $R_n(x)$ $(n \geq 1)$ are real; so $\hat{x}$ is real. The result now follows, since (by the properties of H) $\hat{x}$ is real only if $\hat{z}$ is real.

The following result is used in the verification of orthogonality as well as in the definition of α_2.

Lemma 4.14. The zeros of $P(z)$ in the real interval $(-1,1)$ are simple.

Proof. Let $P(\hat{z}) = 0$ with $\hat{z} \in (-1,1)$, and suppose, contrary to the assertion of the lemma, that $P'(\hat{z}) = 0$. Recall that $\hat{z} \neq 0$ (again see the remarks following Definition 4.1). By (27) and the fact that $P(\hat{z}) = 0$,

$$R_n\left(H(\hat{z})\right) = \frac{\hat{z}^{n+1}\ P(\hat{z}^{-1}) - \hat{z}^{-(n+1)}\ P(\hat{z})}{\hat{z} - \hat{z}^{-1}}$$

$$= \frac{\hat{z}^{n+1}\ P(\hat{z}^{-1})}{\hat{z} - \hat{z}^{-1}}\ , \quad n \geq 2N.$$

Hence, since $|\hat{z}| < 1$,

$$\lim_{n\to\infty} R_n\left(H(\hat{z})\right) = 0. \tag{33}$$

By a direct computation using (27),

$$R_n'\left(H(z)\right)H'(z) =$$

$$\frac{(n+1)z^nP(z^{-1}) - z^{n-1}P'(z^{-1}) + (n+1)z^{-(n+2)}P(z) - z^{-(n+1)}P'(z)}{z - z^{-1}}$$

$$- \frac{(1+z^{-2})[z^{n+1}P(z^{-1})-z^{-(n+1)}P(z)]}{(z-z^{-1})^2} \tag{34}$$

for $0 < |z| < 1$, $n \geq 2N$. Therefore, by (34) and the assumption that $P(\hat{z}) = P'(\hat{z}) = 0$,

$$R_n'\left(H(\hat{z})\right) = \frac{1}{H'(\hat{z})(\hat{z}-\hat{z}^{-1})^2}\ \{(\hat{z}-\hat{z}^{-1})[(n+1)\hat{z}^nP(\hat{z}^{-1})-\hat{z}^{n-1}P'(\hat{z}^{-1})]$$

$$- (1+\hat{z}^{-2})\hat{z}^{n+1}P(\hat{z}^{-1})\}, \quad n\geq 2N. \tag{35}$$

Hence, since $|\hat{z}| < 1$,

$$\lim_{n\to\infty} R_n'\big(H(\hat{z})\big) = 0. \tag{36}$$

From the Christoffel-Darboux identity [19, p.43] and recurrence (R), it can be shown that

$$\frac{1}{c_0\cdots c_N}\,[R_{n+1}'\big(H(\hat{z})\big)R_n\big(H(\hat{z})\big)-R_{n+1}\big(H(\hat{z})\big)R_n'\big(H(\hat{z})\big)]$$

$$= a_0 \sum_{j=0}^{n} \lambda_j [R_j\big(H(\hat{z})\big)]^2, \quad n\geq N-1,$$

where $\lambda_j > 0$ for all $j \geq 0$. Since the limit (as $n\to\infty$) of the left side of the preceding equation is 0 by (33) and (36),

$$a_0 \sum_{j=0}^{\infty} \lambda_j [R_j\big(H(\hat{z})\big)]^2 = 0.$$

Therefore, since $a_0 \neq 0$ and $\lambda_j > 0$,

$$R_j\big(H(\hat{z})\big) = 0$$

for all $j \geq 0$. This is impossible--in particular, since $R_0(x) \equiv 1$. Hence $P'(\hat{z}) \neq 0$. This concludes the proof.

The next two results show that whenever $P(z)$ has zeros in $(-1,1)$, the step function α_2 is defined and the jumps in α_2 are positive.

Lemma 4.16. If $P(\hat{z}) = 0$ with $\hat{z} \in (-1,1)$, then $P(\hat{z}^{-1}) \neq 0$.

Proof. If $P(\hat{z}) = 0$ *and* $P(\hat{z}^{-1}) = 0$, then by (27)

$$R_n\big(H(\hat{z})\big) = \frac{\hat{z}^{n+1}P(\hat{z}^{-1}) - \hat{z}^{-(n+1)}P(\hat{z})}{\hat{z} - \hat{z}^{-1}} = 0, \quad n \geq 2N,$$

a conclusion which is impossible because of the interlacing property of the zeros of $R_n(x)$ $(n \geq 1)$. Hence, $P(\hat{z}^{-1}) \neq 0$.

Lemma 4.17. If $P(\hat{z}) = 0$ with $\hat{z} \in (-1,1)$, then

$$\hat{z}P(\hat{z}^{-1})P'(\hat{z}) > 0.$$

The proof of this lemma is lengthy and is given in the Appendix. It should be noted at this point that the numbers $x_j = H(z_j)$, $j=1,\cdots,p$ (as in Definition 4.4), are limits of certain sequences of zeros of $\{R_n(x)\}$, as described by Lemma A.2 of the Appendix (cf. Martens' result discussed at the beginning of this chapter).

Consideration is now given to the case in which $P(z)$ has zeros on $|z| = 1$. The following two lemmas show that 1 and -1 are the only possibilities and that whenever either of these is a zero of $P(z)$, it is a simple zero.

Lemma 4.18. If z_0 is a complex number with $|z_0| = 1$, and if $P(z_0) = 0$, then $z_0 = 1$ or $z_0 = -1$.

Proof. If $|z_0| = 1$, then $\bar{z}_0 = z_0^{-1}$. Now $P(z)$ has real coefficients; so

$$0 = P(z_0) = P(\bar{z}_0) = P(z_0^{-1}).$$

Let $x_0 = \frac{1}{2}(z_0+z_0^{-1})$. By Equation (29),

$$R_n(x_0) = \frac{z_0^{n+1}P(z_0^{-1}) - z_0^{-(n+1)}P(z_0)}{z_0 - z_0^{-1}} = 0, \quad n \geq 2N,$$

unless $z_0 = 1$ or $z_0 = -1$. This conclusion cannot hold, however, by the interlacing property of the zeros of $\{R_n(x)\}$. Hence $z_0 = 1$ or $z_0 = -1$.

Lemma 4.19. If $P(-1) = 0$, then $P'(-1) \neq 0$; if $P(1) = 0$, then $P'(1) \neq 0$.

Proof. It is first noted, by (8), that

$$Q_j(-1) = \lim_{\theta\to\pi} Q_j(\cos\theta) = \lim_{\theta\to\pi} \frac{\sin(j+1)\theta}{\sin\theta} = (-1)^j(j+1) \tag{37}$$

and

$$Q_j(1) = \lim_{\theta\to 0} Q_j(\cos\theta) = \lim_{\theta\to 0} \frac{\sin(j+1)\theta}{\sin\theta} = j + 1 \tag{38}$$

for all $j \geq 0$. By (19), (37), and the definition of $P(z)$,

$$\begin{aligned} R_n(-1) &= \sum_{\ell=0}^{2N} \beta_\ell Q_{n-\ell}(-1) \\ &= (-1)^n \sum_{\ell=0}^{2N} (-1)^\ell (n-\ell+1)\beta_\ell \\ &= (-1)^n \left[(n+1) \sum_{\ell=0}^{2N} \beta_\ell(-1)^\ell + \sum_{\ell=0}^{2N} \ell\beta_\ell(-1)^{\ell-1}\right] \end{aligned}$$

$$= (-1)^n [(n+1)P(-1)+P'(-1)], \quad n\geq 2N .$$

Suppose that $P(-1) = 0$. Then

$$R_n(-1) = (-1)^{n+1}P'(-1), \quad n\geq 2N.$$

If one supposes also that $P'(-1) = 0$, then -1 is a zero of $R_n(x)$ for all $n \geq 2N$. This is impossible. Hence $P'(-1) \neq 0$ when $P(-1) = 0$. Likewise, by way of (38),

$$R_n(1) = (n+1)P(1) - P'(1),$$

and a similar contradiction arises if it is assumed that $P(1) = P'(1) = 0$. This concludes the proof.

In preparation for the statement of the next lemma, recall that $S(x)$ (Definition 4.2 and Equation (13)) is nonnegative on $[-1,1]$ and that the zeros of $S(x)$ in $[-1,1]$ correspond to zeros of $P(z)$ on $|z| = 1$--i.e., $S(x_0) = 0$ for $x_0 \in [-1,1]$ if and only if $P(e^{i\theta_0}) = 0$, where $x_0 = \cos \theta_0$. It follows from Lemma 4.18 that $S(x) > 0$ on $[-1,1]$ if $P(1) \neq 0$ and $P(-1) \neq 0$ and hence $\int_{-1}^{1} \frac{w_Q(x)}{S(x)}\, dx$ (see Definition 4.3) exists if $P(1) \neq 0$ and $P(-1) \neq 0$. Moreover, $\frac{w_Q(x)}{S(x)} > 0$ on $[-1,1]$. Recall also (Equation (13)) that $S(1) = 0$ if and only if $P(1) = 0$ and that $S(-1) = 0$ if and only if $P(-1) = 0$. By Lemmas 4.18 and 4.19 there are only three possibilities for $P(z)$ if $P(1) = 0$ or $P(-1) = 0$:

$$\text{(i)} \quad P(z) = (z-1)\hat{P}_1(z),$$

$$\text{(ii)} \quad P(z) = (z+1)\hat{P}_2(z), \tag{39}$$

or

$$\text{(iii)} \quad P(z) = (z^2-1)\hat{P}_3(z),$$

where $\hat{P}_j(z)$ $(j=1,2,3)$ does not have a zero on the unit circle $|z| = 1$. The specific possibilities for $S(x)$ when $P(1) = 0$ or $P(-1) = 0$ can now be determined. Suppose first that $P(1) = 0$ and $P(-1) \neq 0$. Then $P(z)$ is given by (39(i)). By (13)

$$\begin{aligned} S(x) &= |P(e^{i\theta})|^2 \\ &= |e^{i\theta}-1|^2 |\hat{P}_1(e^{i\theta})|^2 \\ &= 2(1-\cos\theta)|\hat{P}_1(e^{i\theta})|^2 \\ &= 2(1-x)S_1(x), \end{aligned}$$

where $S_1(x) \overset{d}{=} |\hat{P}_1(e^{i\theta})|^2$ $(x=\cos\theta)$. The argument given at the beginning of this paragraph for $S(x)$ can be applied to $S_1(x)$ to conclude that $S_1(x) > 0$ for $-1 \leq x \leq 1$, since $\hat{P}_1(z)$ has no zeros on the unit circle. Now consider $\frac{w_Q}{S}$ (as in Definition 4.3):

$$\frac{w_Q(x)}{S(x)} = \frac{\frac{2}{\pi}(1-x^2)^{1/2}}{2(1-x)S_1(x)} = \frac{\frac{1}{\pi}(1-x)^{-1/2}(1+x)^{1/2}}{S_1(x)} .$$

Since $S_1(x) > 0$ on $[-1,1]$ and since $w_1(x) = \frac{1}{\pi}(1-x)^{-1/2}(1+x)^{1/2}$ is Riemann integrable (improperly) on $[-1,1]$, $\int_{-1}^{1} \frac{w_Q(x)}{S(x)}\,dx$ exists. Moreover, $\frac{w_Q(x)}{S(x)} > 0$ on $(-1,1)$.

The other two cases of (39) can be handled similarly, and the results can be summarized as follows.

Lemma 4.20. If $P(1) \neq 0$ and $P(-1) \neq 0$, then $\frac{w_Q(x)}{S(x)} > 0$ on $[-1,1]$, and $\int_{-1}^{1} \frac{w_Q(x)}{S(x)}\,dx$ exists. If $P(1) = 0$ or $P(-1) = 0$, there are three possibilities:

(i) $P(z) = (z-1)\hat{P}_1(z)$, in which case

$$S(x) = 2(1-x)S_1(x),$$

(ii) $P(z) = (z+1)\hat{P}_2(z)$, in which case

$$S(x) = 2(1+x)S_2(x),$$

(iii) $P(z) = (z^2-1)\hat{P}_3(z)$, in which case

$$S(x) = 4(1-x^2)S_3(x),$$

where $\hat{P}_j(z)$ has no zeros on the unit circle $|z| = 1$, and

$$S_j(x) \overset{d}{=} |\hat{P}_j(e^{i\theta})|^2 > 0 \quad (x=\cos\theta;\ j=1,2,3).$$

Moreover, $\frac{w_Q}{S} = \frac{w_j}{S_j}$, where for $-1 < x < 1$

$$w_1(x) = \frac{1}{\pi}(1-x)^{-1/2}(1+x)^{1/2},$$

$$w_2(x) = \frac{1}{\pi}(1-x)^{1/2}(1+x)^{-1/2}, \tag{40}$$

$$w_3(x) = \frac{1}{2\pi}(1-x^2)^{-1/2},$$

so that in each of the three possible cases $\frac{w_Q(x)}{S(x)} > 0$ on $(-1,1)$ and $\int_{-1}^{1} \frac{w_Q(x)}{S(x)}\,dx$ exists.

Verification of Orthogonality when $P(1) \neq 0$ and $P(-1) \neq 0$

Suppose that $P(1) \neq 0$ and $P(-1) \neq 0$. As stated in the introductory remarks of the preceding section, $\alpha_R = \alpha_1 + \alpha_2$ is a distribution function, where α_1 and α_2 are defined by (15) and (16) (or (17)), respectively. By Theorem 3.13, orthogonality of $\{R_n(x)\}$ with respect to $d\alpha_R(x)$ is established if the relations

$$\int_{-\infty}^{\infty} R_n(x)Q_\nu(x)d\alpha_R(x) = \delta(n,\nu)\gamma_n, \quad \nu\le n, \tag{41}$$

where $\gamma_n \neq 0$ $(n\ge 2N)$, are shown to hold for all $n \ge 2N$. By the definition of α_R,

$$\int_{-\infty}^{\infty} R_n(x)Q_\nu(x)d\alpha_R(x) = \int_{-\infty}^{\infty} R_n(x)Q_\nu(x)d\alpha_1(x) + \int_{-\infty}^{\infty} R_n(x)Q_\nu(x)d\alpha_2(x). \qquad (42)$$

The first integral on the right side of Equation (42) is evaluated first. By the definition of α_1,

$$\int_{-\infty}^{\infty} R_n(x)Q_\nu(x)d\alpha_1(x) = \int_{-1}^{1} \frac{R_n(x)Q_\nu(x)w_Q(x)}{S(x)}\, dx \stackrel{d}{=} I(n,\nu)$$

for all $n \geq 2N$, $\nu \leq n$. Then by (9)

$$\begin{aligned} I(n,\nu) &= \int_0^\pi \frac{R_n(\cos\theta)Q_\nu(\cos\theta)w_Q(\cos\theta)}{S(\cos\theta)} \sin\theta\, d\theta \\ &= \frac{2}{\pi}\int_0^\pi \frac{R_n(\cos\theta)Q_\nu(\cos\theta)\sin^2\theta}{S(\cos\theta)}\, d\theta \\ &= \frac{2}{\pi}\int_{-\pi}^0 \frac{R_n(\cos\theta)Q_\nu(\cos\theta)\sin^2\theta}{S(\cos\theta)}\, d\theta. \end{aligned}$$

Therefore, by Theorem 4.9 (Equation (25)) and (8)

$$\begin{aligned} I(n,\nu) &= \frac{1}{\pi}\int_{-\pi}^{\pi} \frac{R_n(\cos\theta)Q_\nu(\cos\theta)\sin^2\theta}{S(\cos\theta)}\, d\theta \\ &= \frac{1}{\pi}\int_{-\pi}^{\pi} \frac{Im\{e^{i(n+1)\theta}P(e^{-i\theta})\}\sin(\nu+1)\theta}{S(\cos\theta)}\, d\theta \\ &= \frac{1}{\pi}\, Im\left\{\int_{-\pi}^{\pi} \frac{e^{i(n+1)\theta}P(e^{-i\theta})\sin(\nu+1)\theta}{S(\cos\theta)}\, d\theta\right\}. \end{aligned}$$

Now (13) and conversion to a contour integral yield

$$I(n,\nu) = \frac{1}{\pi}\, Im\left\{\int_{-\pi}^{\pi} \frac{e^{i(n+1)\theta}\sin(\nu+1)\theta}{P(e^{i\theta})}\, d\theta\right\}$$

$$= -\frac{1}{2\pi}\, Im\left\{\int_{|z|=1} \frac{z^n(z^{\nu+1}-z^{-(\nu+1)})}{P(z)}\, dz\right\}, \quad \begin{matrix} n\geq 2N, \\ \nu\leq n, \end{matrix} \tag{43}$$

or

$$I(n,\nu) = -\frac{1}{2\pi}\, Im\left\{\int_{|z|=1} \frac{z^{n+\nu+1}}{P(z)}\, dz - \int_{|z|=1} \frac{z^{n-\nu-1}}{P(z)}\, dz\right\}, \quad \begin{matrix} n\geq 2N, \\ \nu\leq n. \end{matrix} \tag{44}$$

There are two cases to be considered.

Case 1. Suppose that $P(z)$ has no zeros in $(-1,1)$. Then it follows from Corollary 4.13 that $P(z)$ has no zeros in $|z| < 1$. Moreover, since $P(1) \neq 0$ and $P(-1) \neq 0$, it follows from Lemma 4.16 that $P(z)$ has no zeros on $|z| = 1$. These facts together with the fact that $n + \nu + 1 > 1$ imply that the integrand of the first integral in braces in (44) is analytic on $|z| \leq 1$. Hence, this equation reduces to

$$I(n,\nu) = \frac{1}{2\pi}\, Im\left\{\int_{|z|=1} \frac{z^{n-\nu-1}}{P(z)}\, dz\right\}. \tag{45}$$

Also, if $\nu < n$, the exponent $n - \nu - 1$ in (45) is nonnegative so that

$$I(n,\nu) = 0, \quad n\geq 2N,\ \nu<n.$$

For $\nu = n$, Equation (45) and the fact that $P(z)$ has real coefficients give

$$I(n,n) = \frac{1}{2\pi} \mathit{Im} \left\{ \int_{|z|=1} \frac{1}{zP(z)} \, dz \right\}$$

$$= \frac{1}{2\pi} \mathit{Im} \left\{ 2\pi i \cdot \frac{1}{P(0)} \right\}$$

$$= \frac{1}{P(0)} \neq 0 .$$

Hence $I(n,\nu) = \delta(n,\nu) \frac{1}{P(0)}$ $(n \geq 2N,\ \nu \leq n)$. But the second integral on the right side of (42) is zero ($\alpha_2 = 0$ in this case by Definition 4.4). So (41) is verified in case $P(z)$ has no zeros in $(-1,1)$.

Case 2. Suppose that $P(z)$ has zeros $z_1, \cdots, z_p$ in $(-1,1)$. It follows from Corollary 4.13 that these zeros are the only zeros of $P(z)$ in $|z| < 1$. Since $P(1) \neq 0$ and $P(-1) \neq 0$, Lemma 4.16 implies that $P(z)$ has no zeros on $|z| = 1$. Hence, the integrand of the integral in Equation (43) is analytic on $|z| = 1$; it has singularities at $z_1, \cdots, z_p$; and, if $\nu = n$, there is an additional singularity at 0. All these singularities are *simple* poles ($z_1, \cdots, z_p$ are simple by Lemma 4.14). Hence

$$\int_{|z|=1} \frac{z^n(z^{\nu+1} - z^{-(\nu+1)})}{P(z)} \, dz = 2\pi i \sum_{j=1}^{p} \mathrm{Res} \left\{ \frac{z^n(z^{\nu+1} - z^{-(\nu+1)})}{P(z)} ;\ z_j \right\}$$

$$+ 2\pi i \, \mathrm{Res} \left\{ \frac{-1}{zP(z)} ;\ 0 \right\} \delta(n,\nu)$$

$$= 2\pi i \sum_{j=1}^{p} \frac{z_j^n\left(z_j^{\nu+1}-z_j^{-(\nu+1)}\right)}{P'(z_j)} - \frac{2\pi i}{P(0)}\,\delta(n,\nu).$$

From this result, Equation (43), and the facts that $z_1,\cdots,z_p$ are real and that P(z) has real coefficients,

$$I(n,\nu) = -\sum_{j=1}^{p} \frac{z_j^n\left(z_j^{\nu+1}-z_j^{-(\nu+1)}\right)}{P'(z_j)} + \frac{1}{P(0)}\,\delta(n,\nu), \quad n\geq 2N,\ \nu\leq n. \qquad (46)$$

The second integral on the right side of (42) is now evaluated. It is supposed that $z_1,\cdots,z_p$ and $x_1,\cdots,x_p$ are as in Definition 4.4.

By (27), the definition of x_j, and the fact that $P(z_j) = 0$ $(1\leq j\leq p)$,

$$R_n(x_j) = R_n\left(H(z_j)\right) = \frac{z_j^{n+1}P(z_j^{-1})}{z_j - z_j^{-1}}, \quad 1\leq j\leq p,\ n\geq 2N. \qquad (47)$$

Also, by (28),

$$Q_\nu(x_j) = Q_\nu\left(\frac{z_j+z_j^{-1}}{2}\right) = \frac{z_j^{\nu+1}-z_j^{-(\nu+1)}}{z_j - z_j^{-1}}, \quad 1\leq j\leq p,\ \nu\geq 0.$$

The definition of α_2 (Equation (16)) now yields

$$\int_{-\infty}^{\infty} R_n(x)Q_\nu(x)\,d\alpha_2(x) = \sum_{j=1}^{p} R_n(x_j)Q_\nu(x_j)\left[\frac{(z_j-z_j^{-1})^2}{z_jP'(z_j)P(z_j^{-1})}\right]$$

$$= \sum_{j=1}^{p} \frac{z_j^n\left(z_j^{\nu+1}-z_j^{-(\nu+1)}\right)}{P'(z_j)}, \quad n\geq 2N,\ \nu\leq n. \tag{48}$$

When results (46) and (48) are substituted into (42), the result

$$\int_{-\infty}^{\infty} R_n(x)Q_\nu(x)d\alpha_R(x) = \frac{1}{P(0)}\,\delta(n,\nu), \quad n\geq 2N,\ \nu\leq n$$

is obtained. Thus (41) is verified in case $P(z)$ has zeros in $(-1,1)$. This concludes the verification of orthogonality when $P(1) \neq 0$ and $P(-1) \neq 0$.

Note that in both case 1 and case 2

$$\int_{-\infty}^{\infty} R_n(x)Q_n(x)d\alpha_R(x) = \frac{1}{P(0)}, \quad n\geq 2N. \tag{49}$$

This result will be useful when the question of normalization is discussed in section 6.

Verification of Orthogonality when $P(1) = 0$ or $P(-1) = 0$

Suppose first that $P(1) = 0$ and $P(-1) \neq 0$. By Lemma 4.20, $\frac{w_Q(x)}{S(x)} = \frac{w_1(x)}{S_1(x)}$, where $P(z) = (z-1)\hat{P}_1(z)$, $S_1(x) = |\hat{P}_1(e^{i\theta})|^2$ $(x=\cos\theta)$, and $w_1(x) = \frac{1}{\pi}(1-x)^{-1/2}(1+x)^{1/2}$, $-1 < x < 1$. w_1 is the weight function which gives a normalized distribution for the sequence $\{H_n(x)\}$ of orthogonal polynomials, where

$$H_n(x) = \frac{\cos\left(n + \frac{1}{2}\right)\theta}{\cos \frac{1}{2}\theta}, \quad n\geq 0,\ x=\cos\theta \tag{50}$$

(except for a factor depending on n but not on x, $H_n(x)$ $(n\geq 0)$ is the Jacobi polynomial $P_n^{(-1/2,1/2)}(x)$ [19, pp.58-60]). It is convenient to use these polynomials in the orthogonality proof.

As stated in the introductory remarks of section 3, $\alpha_R = \alpha_1 + \alpha_2$ is a distribution function. By Theorem 3.13 it suffices to show that the relations

$$\int_{-\infty}^{\infty} R_n(x)H_\nu(x)d\alpha_R(x) = \delta(n,\nu)\gamma_n, \quad \nu\leq n, \tag{51}$$

where $\gamma_n \neq 0$ $(n\geq 2N)$, hold for $n \geq 2N$. By the definition of α_R,

$$\int_{-\infty}^{\infty} R_n(x)H_\nu(x)d\alpha_R(x) = \int_{-\infty}^{\infty} R_n(x)H_\nu(x)d\alpha_1(x) + \int_{-\infty}^{\infty} R_n(x)H_\nu(x)d\alpha_2(x). \tag{52}$$

The first integral on the right side of Equation (52) is evaluated first. By the definition of α_1 and Lemma 4.20 (as noted in the introductory remarks of this section),

$$\int_{-\infty}^{\infty} R_n(x)H_\nu(x)d\alpha_1(x) = \frac{1}{\pi}\int_{-1}^{1} \frac{R_n(x)H_\nu(x)(1-x)^{-1/2}(1+x)^{1/2}}{S_1(x)}\,dx \stackrel{d}{=} I_1\,(n,\nu)$$

for $n \geq 2N$, $\nu \leq n$. A routine change of variable and use of (25), (50), and Lemma 4.20 lead to

$$I_1(n,\nu) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{1}{\sin\theta} \frac{Im\{e^{i(n+1)\theta}P(e^{-i\theta})\}\cos\left(\nu+\frac{1}{2}\right)\theta(1+\cos\theta)}{|\hat{P}_1(e^{i\theta})|^2\cos\frac{1}{2}\theta}\,d\theta$$

$$= \frac{1}{2\pi}\, Im\left\{\int_{-\pi}^{\pi} \frac{e^{i(n+1)\theta}\cos\left(\nu+\frac{1}{2}\right)\theta}{\sin\frac{1}{2}\theta} \frac{P(e^{-i\theta})}{|\hat{P}_1(e^{i\theta})|^2}\,d\theta\right\}$$

$$= \frac{1}{2\pi}\, Im\left\{\int_{-\pi}^{\pi} \frac{e^{i(n+1)\theta}\left[e^{i\left(\nu+\frac{1}{2}\right)\theta}+e^{-i\left(\nu+\frac{1}{2}\right)\theta}\right]}{e^{i\frac{\theta}{2}}-e^{-i\frac{\theta}{2}}} \frac{\left(e^{-i\theta}-1\right)}{\hat{P}_1(e^{i\theta})}\,i\,d\theta\right\}.$$

Further simplification and conversion to a contour integral yield

$$I_1(n,\nu) = -\frac{1}{2\pi}\, Im\left\{\int_{-\pi}^{\pi} \frac{e^{i(n+1)\theta}\left(e^{i\nu\theta}+e^{-i(\nu+1)\theta}\right)}{\hat{P}_1(e^{i\theta})}\,i\,d\theta\right\}$$

$$= -\frac{1}{2\pi}\, Im\left\{\int_{|z|=1} \frac{z^n(z^\nu+z^{-(\nu+1)})}{\hat{P}_1(z)}\,dz\right\},\quad n\geq 2N,\ \nu\leq n. \tag{53}$$

Note that $\hat{P}_1(z)$ has no zeros on $|z| = 1$ by Lemma 4.20. There are two cases to be considered.

Case 1. Suppose that $P(z)$ (and, hence, $\hat{P}_1(z)$) has no zeros in $(-1,1)$. Then, by Corollary 4.13, $P(z)$ has no zeros in $|z| < 1$. Equation (53) gives

$$I_1(n,\nu) = -\frac{1}{2\pi} Im \left\{ \int_{|z|=1} \frac{z^{n-\nu-1}}{\hat{P}_1(z)} dz \right\}, \quad n \geq 2N, \ \nu \leq n$$

$$= -\frac{1}{\hat{P}_1(0)} \ \delta(n,\nu), \quad n \geq 2N, \ \nu \leq n,$$

as for case 1 in the preceding section. Since the second integral on the right side of (52) is zero ($\alpha_2 = 0$), (51) is verified in case P(z) has no zeros in (-1,1).

Case 2. P(z) (and, hence, $\hat{P}_1(z)$) has zeros $z_1, \cdots, z_p$ in (-1,1). As in the proof of the preceding section (case 2), the fact that $z_1, \cdots, z_p$ are real and simple, the fact that $\hat{P}_1(z)$ has real coefficients, and (53) yield

$$I_1(n,\nu) = -\sum_{j=1}^{p} \frac{z_j^n \left(z_j^\nu + z_j^{-(\nu+1)}\right)}{\hat{P}_1'(z_j)} - \delta(n,\nu) \frac{1}{\hat{P}_1(0)}, \quad n \geq 2N, \ \nu \leq n. \tag{54}$$

By the definition of α_2 (Equation (16)), the second integral on the right side of (52) becomes

$$\int_{-\infty}^{\infty} R_n(x) H_\nu(x) d\alpha_2(x) = \sum_{j=1}^{p} R_n(x_j) H_\nu(x_j) \frac{(z_j - z_j^{-1})^2}{z_j P(z_j^{-1}) P'(z_j)}, \quad n \geq 2N, \ \nu \leq n. \tag{55}$$

Like the representation (28) for $Q_\nu(x)$, a representation for $H_\nu(x)$ can be obtained from (50); namely,

$$H_\nu\left(\frac{1}{2}(z+z^{-1})\right) = \frac{z^\nu + z^{-(\nu+1)}}{1+z^{-1}}, \quad \nu\geq 0,\ z\neq 0,$$

from which it follows that

$$H_\nu(x_j) = H_\nu\left(\frac{1}{2}(z_j+z_j^{-1})\right) = \frac{z_j^\nu + z_j^{-(\nu+1)}}{1+z_j^{-1}}, \quad \nu\geq 0,\ 1\leq j\leq p.$$

This result and Equation (47) are used to reduce the right side of (55).

$$\sum_{j=1}^{p} R_n(x_j)H_\nu(x_j)\frac{(z_j-z_j^{-1})^2}{z_jP'(z_j)P(z_j^{-1})} = \sum_{j=1}^{p}\frac{z_j^n\left(z_j^\nu+z_j^{-(\nu+1)}\right)(z_j-z_j^{-1})}{(1+z_j^{-1})P'(z_j)}. \tag{56}$$

But

$$P(z) = (z-1)\hat{P}_1(z).$$

So,

$$P'(z_j) = (z_j-1)\hat{P}_1'(z_j), \quad 1\leq j\leq p,$$

since $\hat{P}_1(z_j) = 0$ $(1\leq j\leq p)$. Hence, the right side of (56) becomes

$\sum_{j=1}^{p}\frac{z_j^n\left(z_j^\nu+z_j^{-(\nu+1)}\right)}{\hat{P}_1'(z_j)}$, which is also the right side of (55). From (54)

and (52) it then follows that

$$\int_{-\infty}^{\infty} R_n(x)H_\nu(x)d\alpha_R(x) = -\delta(n,\nu)\,\frac{1}{\hat{P}_1(0)}\,, \quad \nu\leq n,\ n\geq 2N.$$

Thus, (51) is verified in case $P(z)$ has zeros in $(-1,1)$. This concludes the proof of orthogonality when $P(1) = 0$, $P(-1) \neq 0$.

Note that in both cases above,

$$\int_{-\infty}^{\infty} R_n(x)H_n(x)d\alpha_R(x) = -\frac{1}{\hat{P}_1(0)}\,, \quad n\geq 2N. \tag{57}$$

There are two other possibilities for $P(z)$ to be considered in this section: the case in which $P(-1) = 0$ and $P(1) \neq 0$ and the case in which $P(1) = P(-1) = 0$. In both instances the proof of orthogonality is similar to the one just completed. If $P(-1) = 0$ and $P(1) \neq 0$, $\frac{w_Q}{S} = \frac{w_2}{S_2}$ (by Lemma 4.20), where w_2 is a weight function on $(-1,1)$ for the sequence $\{M_n(x)\}$ of orthogonal polynomials given by

$$M_n(x) = \frac{\sin\left(n + \frac{1}{2}\right)\theta}{\sin\frac{\theta}{2}}\,, \quad n\geq 0, \quad x=\cos\theta$$

(except for a factor depending on n but not on x, $M_n(x)$ $(n\geq 0)$ is the Jacobi polynomial $P_n^{(1/2,-1/2)}(x)$ [19, pp.58-60]). It is convenient to use $\{M_n(x)\}$ (as $\{H_n(x)\}$ was used in the proof above) to verify that $\{R_n(x)\}$ is orthogonal with respect to $d\alpha_R(x)$. One result established in the proof is

$$\int_{-\infty}^{\infty} R_n(x)M_n(x)d\alpha_R(x) = \frac{1}{\hat{P}_2(0)}, \quad n\geq 2N, \tag{58}$$

where $\hat{P}_2(z)$ is defined in Lemma 4.20. If $P(1) = P(-1) = 0$, $\frac{w_Q}{S} = \frac{w_3}{S_3}$, where w_3 is a weight function for the sequence $\{T_n(x)\}$ of orthogonal polynomials given by

$$T_n(x) = \cos n\theta, \quad n\geq 0, \; x=\cos\theta,$$

which are the Chebyshev polynomials of the first kind [19, pp.58-60]. It is convenient to use $\{T_n(x)\}$ in the proof of orthogonality in this case. One result from the proof is

$$\int_{-\infty}^{\infty} R_n(x)T_n(x)d\alpha_R(x) = -\frac{1}{2\hat{P}_3(0)}, \quad n\geq 2N, \tag{59}$$

where $\hat{P}_3(z)$ is defined in Lemma 4.20. This concludes the discussion of the orthogonality proofs for this section and completes the proof of Theorem 4.5.

As an aside to this section, it is interesting to note the physical chains associated with the sequences $\{H_n(x)\}$, $\{M_n(x)\}$, and $\{T_n(x)\}$, each of which is generated by a recurrence which is a special case of (R). First, the sequence $\{H_n(x)\}$ satisfies the recurrence

$$H_{-1}(x) = 0, \quad H_0(x) = 1,$$

$$H_1(x) = 2x - 1, \tag{H}$$

$$H_{n+1}(x) = 2xH_n(x) - H_{n-1}(x), \quad n \geq 1.$$

It is associated (after the change of variable discussed in Chapter III) with the uniform semi-infinite chain without initial spring (Figure 1(b)), and it also appears in connection with the finitely defective chains without initial springs discussed in Chapter VI. Second, the sequence $\{M_n(x)\}$ satisfies

$$M_{-1}(x) = 0, \quad M_0(x) = 1,$$

$$M_1(x) = 2x + 1,$$

$$M_{n+1}(x) = 2xM_n(x) - M_{n-1}(x), \quad n \geq 1.$$

It is associated (after the change of variable) with the semi-infinite chain shown in Figure 6.

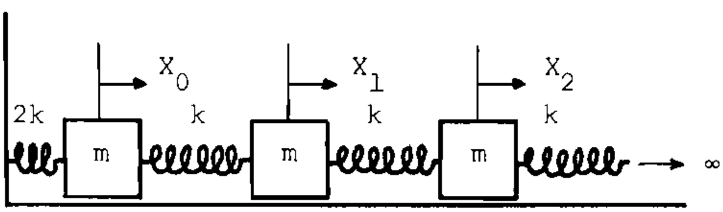


Figure 6. The Semi-Infinite Chain Associated with $\{M_n(x)\}$

Finally, the sequence $\{T_n(x)\}$ satisfies

$$T_{-1}(x) = 0, \quad T_0(x) = 1,$$

$$T_1(x) = x,$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad n\geq 1,$$

and is associated with the semi-infinite chain shown in Figure 7.

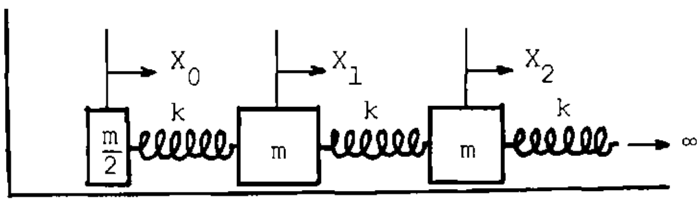


Figure 7. The Semi-Infinite Chain Associated with $\{T_n(x)\}$

Normalization

The problem of obtaining a *normalized* distribution for $\{R_n(x)\}$ is now considered. Let α_R be the distribution function for $\{R_n(x)\}$ given by Theorem 4.5. Then $\alpha_R(x) \to 0$ as $x \to -\infty$. By the remarks following Definition 3.3, if

$$\sigma \overset{d}{=} \int_{-\infty}^{\infty} d\alpha_R(x),$$

then $\frac{1}{\sigma}\,\alpha_R$ gives a normalized distribution. By Theorem 3.12 and recurrence (R), for all $j \geq N-1$,

$$\int_{-\infty}^{\infty} [R_j(x)]^2 d\left(\frac{1}{\sigma}\,\alpha_R\right)(x) = \frac{1}{\sigma} \int_{-\infty}^{\infty} [R_j(x)]^2 d\alpha_R(x)$$

$$= \begin{cases} a_0, & \text{if } N = 1, \\ a_0 c_1 \cdots c_{N-1}, & \text{if } N > 1. \end{cases} \tag{60}$$

Thus, if $\int_{-\infty}^{\infty} [R_{2N}(x)]^2 d\alpha_R(x)$ (for example) were known, σ could be computed from (60). Because of the way in which the orthogonality was verified, there are two cases to be considered in the computation of $\int_{-\infty}^{\infty} [R_{2N}(x)]^2 d\alpha_R(x)$.

Case 1. Suppose that $P(1) \neq 0$ and $P(-1) \neq 0$. By (10), (49) (with $n=2N$), and the definition of $P(z)$,

$$\int_{-\infty}^{\infty} [R_{2N}(x)]^2 d\alpha_R(x) = \int_{-\infty}^{\infty} R_{2N}(x) \sum_{\ell=0}^{2N} \beta_\ell Q_{2N-\ell}(x) d\alpha_R(x)$$

$$= \beta_0 \int_{-\infty}^{\infty} R_{2N}(x) Q_{2N}(x) d\alpha_R(x)$$

$$= \frac{\beta_0}{P(0)}$$

$$= 1.$$

Case 2. Suppose that $P(1) = 0$ or $P(-1) = 0$. First, the case

$P(1) = 0$, $P(-1) \neq 0$ is considered. Note that the sequence $\{H_n(x)\}$ is related to $\{Q_n(x)\}$ by

$$Q_n(x) = H_n(x) + H_{n-1}(x), \quad n\geq 0.$$

Then by (10), (57) (with n=2N), and the definition of P(z),

$$\begin{aligned}\int_{-\infty}^{\infty} [R_{2N}(x)]^2 d\alpha_R(x) &= \beta_0 \int_{-\infty}^{\infty} R_{2N}(x)Q_{2N}(x)d\alpha_R(x) \\ &= \beta_0 \int_{-\infty}^{\infty} R_{2N}(x)[H_{2N}(x)+H_{2N-1}(x)]d\alpha_R(x) \\ &= \beta_0 \int_{-\infty}^{\infty} R_{2N}(x)H_{2N}(x)d\alpha_R(x) \\ &= -\frac{\beta_0}{\hat{P}_1(0)} \\ &= -\frac{P(0)}{\hat{P}_1(0)} .\end{aligned}$$

But $P(z) = (z-1)\hat{P}_1(z)$; so $P(0) = -\hat{P}_1(0)$. Thus, the last relation above gives

$$\int_{-\infty}^{\infty} [R_{2N}(x)]^2 d\alpha_R(x) = 1.$$

The same result can be shown to hold in the other two cases ($P(-1) = 0$, $P(1) \neq 0$ and $P(1) = P(-1) = 0$) by using (58) with the relation

$Q_n(x) = M_n(x) - M_{n-1}(x)$ $(n\geq 0)$ or (59) with the relation $Q_n(x) = 2T_n(x)$ $(n\geq 0)$.

Since

$$\int_{-\infty}^{\infty} [R_{2N}(x)]^2 d\alpha_R(x) = 1$$

under all circumstances, the normalization factor σ can now be computed by using this relation and (60). Thus

$$\sigma \stackrel{d}{=} \int_{-\infty}^{\infty} d\alpha_R(x) = \begin{cases} a_0^{-1}, & \text{if } N=1 \\ (a_0 c_1 \cdots c_{N-1})^{-1}, & \text{if } N>1. \end{cases} \tag{61}$$

CHAPTER V

SOLUTION OF THE BASIC INITIAL-VALUE PROBLEM AND SOME EXAMPLES

In this chapter the procedures developed in Chapter IV are applied to the solution of the basic initial-value problem [IVP] for the finitely defective semi-infinite chain of springs and masses (see Figure 4). A general formula for the solution of [IVP] is developed, and the examples introduced in Chapter II are discussed.

Let $\{P_n(x)\}$ be the sequence of orthogonal polynomials which is associated with the finitely defective semi-infinite chain by Theorem 3.11. Let $\{R_n(x)\}$ be the sequence of orthogonal polynomials generated by the recurrence

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_{n+1}(x) = \left[2\frac{\mu_n}{\lambda_{n+1}}x + \left(1 + \frac{\lambda_n}{\lambda_{n+1}} - \frac{2\mu_n}{\lambda_{n+1}}\right)\right]R_n(x) - \frac{\lambda_n}{\lambda_{n+1}}R_{n-1}(x), \qquad 0 \le n \le N-1, \tag{62}$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad n \ge N,$$

where $\lambda_N \overset{d}{=} 1$. This sequence was called $\{\tilde{P}_n(x)\}$ in Chapter III, and is related to $\{P_n(x)\}$ by

$$P_n\left(-\frac{2k}{m}(x-1)\right) = R_n(x), \quad n\geq 0. \tag{63}$$

As noted in Chapter III, the recurrence generating $\{R_n(x)\}$ is of type (R). For the sequence $\{R_n(x)\}$, let $P(z)$ and α_R be the polynomial and the distribution function determined by the procedures described in Chapter IV. Let

$$\alpha(x) = -\alpha_R\left(-\frac{m}{2k}x + 1\right). \tag{64}$$

Then α is a distribution function, and $\{P_n(x)\}$ is orthogonal with respect to $d\alpha(x)$. Results of W. G. Christian [8] imply that the distribution for $\{P_n(x)\}$ is unique and that its support is contained in the interval $[0,\infty)$; therefore, it follows from (64) that the support of $d\alpha_R(x)$ is contained in $(-\infty,1]$. Furthermore, since the zeros of $P(z)$ in $(-1,0)$ and $(0,1)$ determine points of increase of α_R in $(-\infty,-1)$ and $(1,\infty)$, respectively, $P(z)$ can have no zeros in $(0,1)$. The possibility that $P(1) = 0$ is not precluded.

By Theorem 3.11, a solution of [IVP] is given by

$$X_n(t) = \frac{1}{\sigma}\int_{-\infty}^{\infty} P_n(x)F(x,t)d\alpha(x), \quad n\geq 0,$$

where $\sigma \overset{d}{=} \int_{-\infty}^{\infty} d\alpha(x)$. The remarks in the preceding paragraph and relations (63) and (64) lead to

$$X_n(t) = -\frac{1}{\sigma}\int_0^\infty P_n(x)F(x,t)\,d\alpha(x)$$

$$= \frac{1}{\sigma}\int_{-\infty}^{1} P_n\left(-\frac{2k}{m}(x-1)\right)F\left(-\frac{2k}{m}(x-1),t\right)d\alpha_R(x)$$

$$= \frac{1}{\sigma}\int_{-\infty}^{1} R_n(x)F\left(\frac{2k}{m}(1-x),t\right)d\alpha_R(x), \quad n\geq 0. \tag{65}$$

By Theorem 3.11, for $-\infty<x\leq 1$,

$$F\left(\frac{2k}{m}(1-x),t\right) = \frac{1}{\zeta_r}P_r\left(\frac{2k}{m}(1-x)\right)\left[d_r\cos t\sqrt{\frac{2k}{m}(1-x)}\right.$$

$$\left.+\frac{v_r}{\sqrt{\frac{2k}{m}(1-x)}}\sin t\sqrt{\frac{2k}{m}(1-x)}\right],$$

where

$$\zeta_r \stackrel{d}{=} \frac{1}{\sigma}\int_{-\infty}^{\infty}[P_r(x)]^2 d\alpha(x) = \frac{1}{\sigma}\int_{-\infty}^{\infty}[R_r(x)]^2 d\alpha_R(x), \quad r\geq 0. \tag{66}$$

But $P_r\left(\frac{2k}{m}(1-x)\right) = R_r(x)$; thus (65) becomes

$$X_n(t) = \frac{1}{\sigma\zeta_r}\int_{-\infty}^{1} R_n(x)R_r(x)\left[d_r\cos t\sqrt{\frac{2k}{m}(1-x)}\right.$$

$$+ \frac{v_r}{\sqrt{\frac{2k}{m}(1-x)}} \sin t\sqrt{\frac{2k}{m}(1-x)}\Bigg] d\alpha_R(x). \tag{67}$$

By Equation (61) and recurrence (62)

$$\sigma \overset{d}{=} \int_{-\infty}^{\infty} d\alpha(x) = \int_{-\infty}^{\infty} d\alpha_R(x) = \frac{1}{\mu_0} . \tag{68}$$

Also, by Equation (4) and recurrence (62),

$$\zeta_r = \begin{cases} 1, & r=0 \\ \dfrac{\mu_0}{\mu_r}, & 1 \le r \le N-1 \\ \mu_0, & r \ge N. \end{cases} \tag{69}$$

When information about the distribution $d\alpha_R(x)$ is incorporated in (67), a formula for a solution of [IVP] may be stated as follows.

Theorem 5.1. Let $\{R_n(x)\}$ be the sequence of polynomials generated by (62). Let $P(z)$ be the polynomial associated with $\{R_n(x)\}$ by Definition 4.1. Let σ and ζ_r be given by (68) and (69), respectively. If $P(z)$ has zeros $z_1, \cdots, z_p$ in $(-1,0)$, let $x_\ell = \frac{1}{2}(z_\ell + z_\ell^{-1})$ for $\ell = 1,2,\cdots,p$. Then, a solution of [IVP] is

$$X_n(t) = \frac{2}{\sigma\zeta_r\pi} \int_0^\pi \frac{R_n(\cos\theta)R_r(\cos\theta)\sin^2\theta}{|P(e^{i\theta})|^2} \, d_r\Bigg[\cos\left(2\sqrt{k/m}\; t \sin\frac{\theta}{2}\right)$$

$$+ v_r \frac{\sin\left(2\sqrt{k/m}\ t \sin \frac{\theta}{2}\right)}{2\sqrt{k/m}\ \sin \frac{\theta}{2}} \Bigg] d\theta + Y_n(t), \quad n\geq 0, \tag{70}$$

where

$$Y_n(t) = \begin{cases} 0, & \text{if } P(z) \text{ has no zeros in } (-1,0), \\ \dfrac{1}{\sigma\zeta_r} \displaystyle\sum_{\ell=0}^{p} \left\{ \dfrac{(z_\ell - z_\ell^{-1})^2}{z_\ell P'(z_\ell) P(z_\ell^{-1})} \left[d_r \cos t\sqrt{\dfrac{2k}{m}(1-x_\ell)} \right.\right. & \\ \left.\left. \quad + \dfrac{v_r}{\sqrt{\dfrac{2k}{m}(1-x_\ell)}} \sin t\sqrt{\dfrac{2k}{m}(1-x_\ell)} \right] R_n(x_\ell) R_r(x_\ell) \right\}, & \text{otherwise.} \end{cases}$$

Proof. The result follows from remarks made at the beginning of this chapter, Theorem 4.5, Equation (67), and the substitution $x = \cos\theta$.

Thus, in order to write a solution of [IVP] it suffices to know $\{R_n(\cos\theta)\}$, $P(z)$, whether or not $P(z)$ has zeros in $(-1,0)$ and, if so, the location of such zeros. A useful representation of $R_n(\cos\theta)$ $(n\geq N-1)$ is given by Theorem 4.9; for $0 \leq n < N-1$, the polynomial $R_n(\cos\theta)$ must be determined directly from recurrence (62). It may not be possible to determine the zeros of $P(z)$ explicitly as functions of the μ_i, λ_i $(0\leq i\leq N-1)$ in every case. So it may be necessary sometimes to approximate the zeros of $P(z)$ by numerical techniques.

Three types of defects frequently associated with linear chains were described in Chapter II: the isotope, the hole, and the interstitial. These examples of finitely defective chains are discussed now in greater detail.

The Single Isotope

Consider a semi-infinite chain of springs and masses in which all the spring constants are the same and all the masses are the same except perhaps one of them (see Figure 8). The positive integer N and the positive number μ will be treated as parameters in the succeeding discussion.

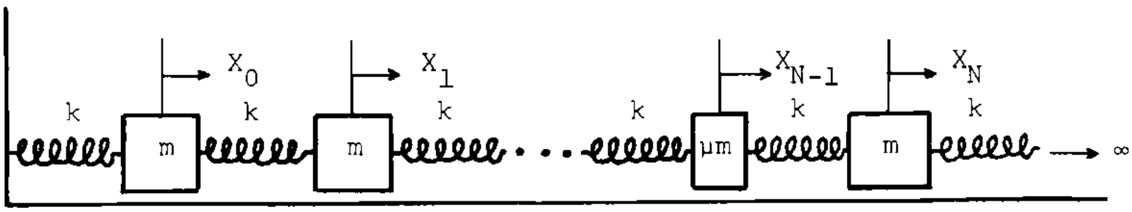


Figure 8. A Semi-Infinite Chain with a Single Isotope

Recurrence (62) becomes

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad 0 \le n \le N-2 \text{ and } n \ge N, \tag{71}$$

$$R_N(x) = [2\mu x+2(1-\mu)]R_{N-1}(x) - R_{N-2}(x).$$

To determine $P(z)$, the expansions of the polynomials $R_n(x)$ as linear combinations of the $Q_j(x)$ are derived. Thus, from (71) and recurrence (Q)

$$R_n(x) = Q_n(x), \quad 0 \le n \le N-1,$$

$$\begin{aligned} R_N(x) &= \mu[2xQ_{N-1}(x)] + 2(1-\mu)Q_{N-1}(x) - Q_{N-2}(x) \\ &= \mu[Q_N(x) + Q_{N-2}(x)] + 2(1-\mu)Q_{N-1}(x) - Q_{N-2}(x) \\ &= \mu Q_N(x) + 2(1-\mu)Q_{N-1}(x) + (\mu-1)Q_{N-2}(x). \end{aligned}$$

Identities (18) and (22) and the above expressions for $R_N(x)$ and $R_{N-1}(x)$ then yield

$$\begin{aligned} R_{2N}(x) &= Q_N(x)R_N(x) - Q_{N-1}(x)R_{N-1}(x) \\ &= Q_N(x)[\mu Q_N(x) + 2(1-\mu)Q_{N-1}(x) + (\mu-1)Q_{N-2}(x)] - Q_{N-1}(x)Q_{N-1}(x) \\ &= \mu \sum_{\ell=0}^{N} Q_{2\ell}(x) + 2(1-\mu) \sum_{\ell=0}^{N-1} Q_{2\ell+1}(x) \\ &\qquad + (\mu-1) \sum_{\ell=0}^{N-2} Q_{2\ell+2}(x) - \sum_{\ell=0}^{N-1} Q_{2\ell}(x) \\ &= \mu Q_{2N}(x) + (\mu-1) \sum_{\ell=0}^{N-1} Q_{2\ell}(x) + 2(1-\mu) \sum_{\ell=0}^{N-1} Q_{2\ell+1}(x) \end{aligned}$$

$$+ (\mu-1) \sum_{\ell=1}^{N-1} Q_{2\ell}(x)$$

$$= \mu Q_{2N}(x) + 2(1-\mu)\left[\sum_{\ell=0}^{N-1} Q_{2\ell+1}(x) - \sum_{\ell=1}^{N-1} Q_{2\ell}(x)\right] + (\mu-1)Q_0(x).$$

The polynomial $P(z)$ is determined from this expansion for $R_{2N}(x)$. Thus, by Definition 4.1,

$$P(z) = (\mu-1)z^{2N} + 2(1-\mu)\left[\sum_{\ell=0}^{N-1} z^{2N-2\ell-1} - \sum_{\ell=1}^{N-1} z^{2N-2\ell}\right] + \mu$$

$$= (\mu-1)z^{2N} + 2(1-\mu) \sum_{\ell=1}^{2N-1} (-1)^{\ell+1} z^{\ell} + \mu. \tag{72}$$

The location of the zeros of $P(z)$ is now examined. For $N = 1$,

$$P(z) = (\mu-1)z^2 + 2(1-\mu)z + \mu,$$

the zeros of which are $1 + (1-\mu)^{-1/2}$ and $1 - (1-\mu)^{-1/2}$, where $\mu \neq 1$. Thus, for $N = 1$, $P(z)$ has no real zeros if $\mu > 1$; $P(z)$ has no zeros in $(-1,0)$ if $\frac{3}{4} \leq \mu < 1$; $P(z)$ has exactly one zero in $(-1,0)$ if $0 < \mu < \frac{3}{4}$; and $P(-1) = 0$ if $\mu = \frac{3}{4}$. For $N = 2$, $P(z)$ is of degree 4 and the zeros of $P(z)$ can be determined explicitly as functions of μ. For $N > 2$, $P(z)$ has degree at least 6; and although for some fixed $N > 2$, it may be possible to determine the zeros explicitly as functions of μ, such an undertaking is not included in the present study. Nevertheless, some information concerning the location of the zeros of $P(z)$ can be adduced. For this purpose, Equation (72) is rewritten as

$$P(z) = (\mu-1)g(z) + 1,^{*} \tag{73}$$

where

$$g(z) \stackrel{d}{=} z^{2N} + 2 \sum_{\ell=1}^{2N-1} (-1)^{\ell} z^{\ell} + 1 = (z-1)^2 \sum_{\ell=0}^{N-1} z^{2\ell}.$$

If z is a zero of $P(z)$, $g(z) \neq 0$ and

$$\mu = 1 - \frac{1}{g(z)} . \tag{74}$$

But $g(z) \geq 0$ for all real z. Hence the above equation implies that $P(z)$ has no real zeros for $\mu > 1$. Furthermore, g is continuous and strictly decreasing on the real interval $(-\infty,0)$; $g(0) = 1$; and $g(z) \to \infty$ as $z \to -\infty$. Therefore, Equation (74) defines μ as a continuous, strictly decreasing function of z on $(-\infty,0)$; moreover, this function assumes every value in (0,1). It follows that (74) also defines z as a continuous function of μ on (0,1) (the main properties of this inverse function are illustrated by Figure 9). By hypothesis, z is a zero of $P(z)$. Hence, for $0 < \mu < 1$, $P(z)$ has exactly one real zero, and this zero lies in the interval $(-\infty,0)$.

---

*The case $\mu = 1$ is dismissed at this point by noting that $P(z) \equiv 1$ for $\mu = 1$. Thus, $d\alpha_R(x) = w_Q(x)dx$, as expected, since $R_n(x) = Q_n(x)$ $(n \geq 0)$ in this case. Hereafter it is assumed that $\mu \neq 1$.

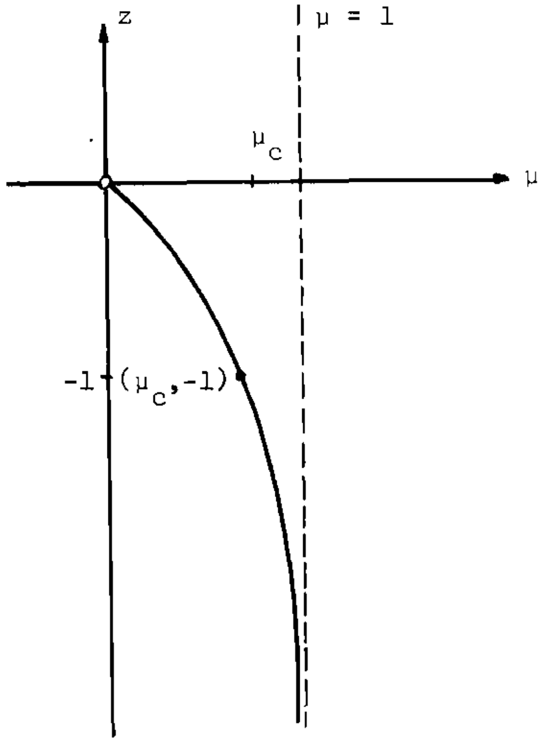


Figure 9. The Negative Real Zero of P(z) for the Single Isotope

It also follows that there is a "critical value" $\mu_c \in (0,1)$, such that if $\mu = \mu_c$, $P(-1) = 0$, and if $0 < \mu < \mu_c$, P(z) has exactly one zero in (-1,0). The number μ_c is determined by

$$0 = P(-1) = (\mu_c - 1) - 2(1-\mu_c)(2N-1) + \mu_c,$$

from Equation (72). Thus,

$$\mu_c = \frac{4N - 1}{4N} .^*$$

A summary of results relevant to the construction of the distribution function α_R for the case of the single isotope can now be given. For fixed $N \geq 1$,

(i) if $\mu > \frac{4N - 1}{4N}$ $(\mu \neq 1)$, $P(z)$ has no zeros in $[-1,0)$; so the support of $d\alpha_R(x)$ is $[-1,1]$, and

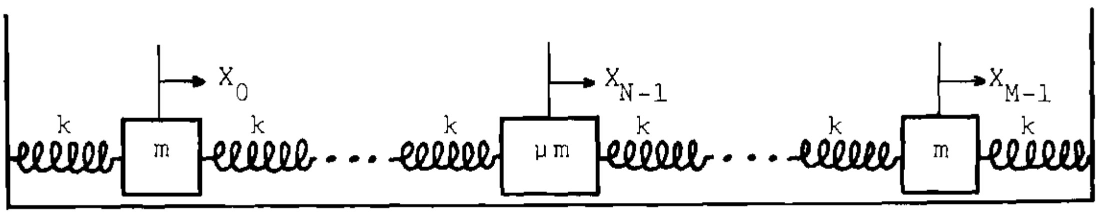
$$d\alpha_R(x) = \frac{w_Q(x)}{S(x)}\,dx = \frac{\frac{2}{\pi}\,(1-x^2)^{1/2}}{S(x)}\,dx;$$

(ii) if $\mu = \frac{4N - 1}{4N}$, $P(-1) = 0$ and $P(z)$ has no zeros in $(-1,0)$ (thus $P(z) = (z+1)\hat{P}_2(z)$, where $\hat{P}_2(z)$ has no zeros in $(-1,0)$); so the support of $d\alpha_R(x)$ is $[-1,1]$, and

$$d\alpha_R(x) = \frac{w_2(x)}{S_2(x)}\,dx = \frac{1}{\pi}\,\frac{(1-x)^{1/2}(1+x)^{-1/2}}{S_2(x)} ,$$

---

*It is interesting to compare this result with a result of W. G. Christian [7], who considered the finite chain (see figure below) of M masses and M + 1 springs in which all the spring constants are the same and all but one of the masses are the same.



Christian found that if $0 < \mu < \mu_c(M) \overset{d}{=} 1 - \frac{M + 1}{4N(M+1-N)}$, all the characteristic frequencies of the system *except one of them* are in the interval $[0, 2\sqrt{k/m}]$. As $M \to \infty$, $\mu_c(M) \to \frac{4N - 1}{4N}$.

where $S_2(x) = |\hat{P}_2(e^{i\theta})|^2$, $x = \cos\theta$;

(iii) if $0 < \mu < \frac{4N-1}{4N}$, $P(z)$ has exactly one zero, z_1, in $(-1,0)$; so $\alpha_R(x) = \alpha_1(x) + \alpha_2(x)$, where the support of $d\alpha_1(x)$ is $[-1,1]$,

$$d\alpha_1(x) = \frac{w_Q(x)}{S(x)}\,dx,$$

and with $x_1 \overset{d}{=} \frac{1}{2}(z_1+z_1^{-1})$,

$$\alpha_2(x) = \begin{cases} 0, & -\infty<x<x_1 \\ \dfrac{(z_1-z_1^{-1})^2}{z_1P(z_1^{-1})P'(z_1)}, & x\geq x_1 \end{cases}$$

(so

$$d\alpha_2(x) = \frac{(z_1-z_1^{-1})^2}{z_1P(z_1^{-1})P'(z_1)}\,\delta(x-x_1)dx).$$

As an example, suppose that $N = 3$. Then, by (73),

$$P(z) = (\mu-1)(z-1)^2(1+z^2+z^4) + 1$$

$$= (\mu-1)\,\frac{z-1}{z+1}\,(z^6-1) + 1. \qquad (75)$$

The coefficient μ is now chosen so that $P(-1/2) = 0$.

Thus,

$$\mu = \frac{125}{189}$$

$(\mu_c = \frac{11}{12}$, in this case), and

$$z_1 = -\frac{1}{2}$$

in the nomenclature of Theorem 5.1. Then x_1, the location of the jump in $\alpha_2(x)$, is given by

$$x_1 = \frac{1}{2}(z_1+z_1^{-1}) = -\frac{5}{4} .$$

Thus, the jump in $\alpha_2(x)$ occurs at $-\frac{2k}{m}\left(-\frac{5}{4}-1\right) = \frac{9}{4}(2k/m)$, and the corresponding frequency is $\frac{3}{2}\sqrt{2k/m}$. The jump $J(x_1)$ is given by

$$J(x_1) = \frac{(z_1-z_1^{-1})^2}{z_1 P(z_1^{-1})P'(z_1)} .$$

From (75),

$$P(z_1^{-1}) = (\mu-1)\frac{z_1^{-1}-1}{z_1^{-1}+1}(z_1^{-6}+1)+1 = -\frac{4097}{63} , \qquad (76)$$

and

$$P'(z_1) = (\mu-1)\left[\frac{6(z_1-1)}{z_1+1}z_1^5 + \frac{2(z_1^6-1)}{(z_1+1)^2}\right] = \frac{52}{21} .$$

Hence,

$$J(x_1) = \frac{11,907}{426,088} \approx 0.028.$$

Now, by (75)

$$P(e^{i\theta}) = (\mu-1)\,\frac{e^{i\theta} - 1}{e^{i\theta} + 1}\,(e^{6i\theta}-1) + 1$$

$$= 1 - 2(\mu-1)\,\frac{\sin\frac{\theta}{2}}{\cos\frac{\theta}{2}}\,\sin 3\theta \cos 3\theta$$

$$+ i\left[-2(\mu-1)\,\frac{\sin\frac{\theta}{2}}{\cos\frac{\theta}{2}}\,\sin^2 3\theta\right].$$

So,

$$|P(e^{i\theta})|^2 = 1 - 4(\mu-1)\,\frac{1-\cos\theta}{\sin\theta}\,\sin 3\theta\cos 3\theta + 4(\mu-1)^2\,\frac{(1-\cos\theta)^2}{\sin^2\theta}\,\sin^2 3\theta$$

$$= 1 + \frac{256}{189}\,(1-\cos\theta)\,\frac{\sin 3\theta}{\sin\theta}\left[\cos 3\theta + \frac{64}{189}\,(1-\cos\theta)\,\frac{\sin 3\theta}{\sin\theta}\right].$$

Though the result is not needed to apply Theorem 5.1, it is noted that the polynomial $S(x)$ can be determined with little difficulty from the last equation with $x = \cos\theta$. The result is

$$S(x) = 1 + \frac{256}{189}(1-x)Q_2(x)\left[\frac{1}{2}Q_3(x) - \frac{1}{2}Q_1(x) + \frac{64}{189}(1-x)Q_2(x)\right]$$

$$= 1 + \frac{256}{189}(1-x)(4x^2-1)\left[4x^3 - 4x + \frac{64}{189}(1-x)(4x^2-1)\right].$$

The distributions $d\alpha_1(x) = \frac{w_Q(x)}{S(x)}dx$ and $d\alpha_2(x)$ associated with this problem are represented in Figures 10 and 11.

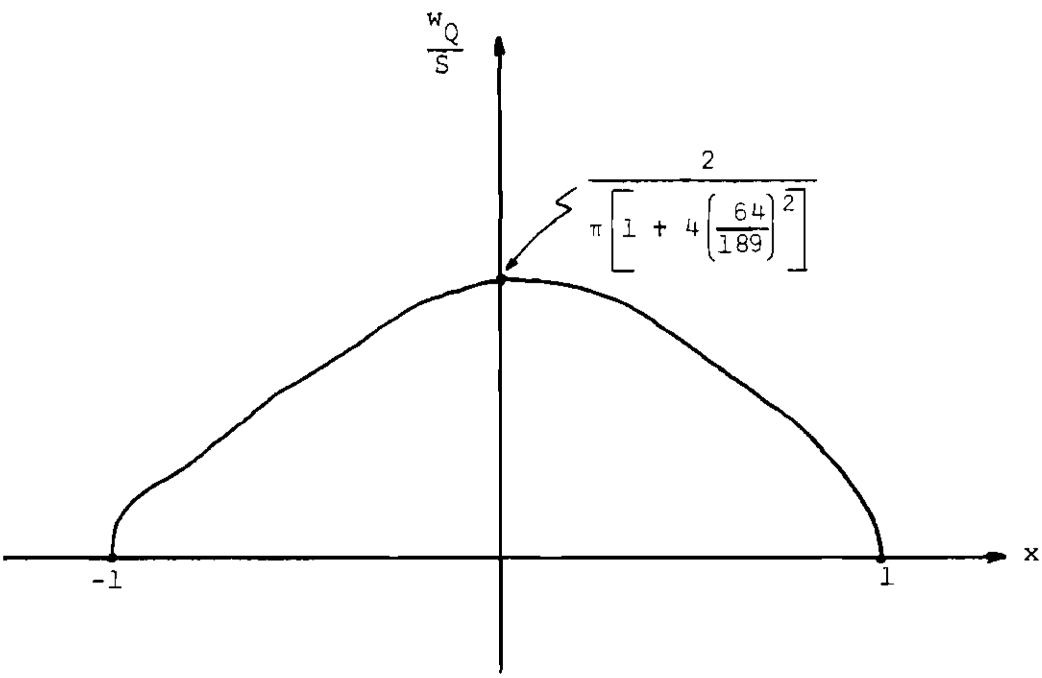


Figure 10. The Weight Function $\frac{w_Q}{S}$

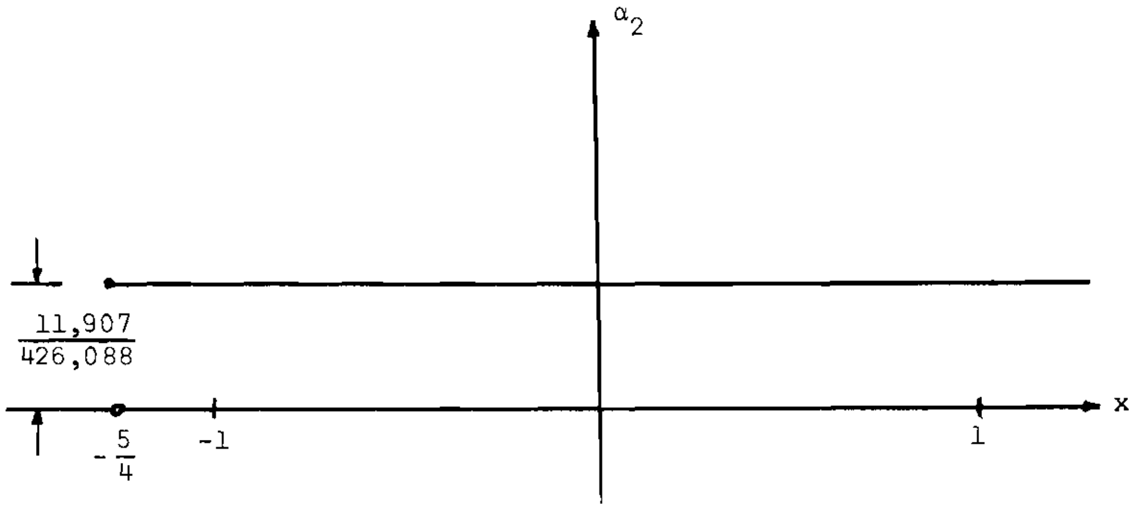


Figure 11. The Distribution Function α_2

Some other information associated with Equation (70) for this problem is now determined. By (68),

$$\sigma = 1,$$

and by (69),

$$\zeta_r = \begin{cases} 1, & r \neq 2 \\ \frac{189}{125}, & r = 2 . \end{cases}$$

The numbers $R_n(x_1) = R_n\left(-\frac{5}{4}\right)$ can be computed from the recurrence for $\{R_n(x)\}$ for $0 \le n \le 2N-1 = 5$. For $n \ge 6$, Equations (47) and (76) give

$$R_n\left(-\frac{5}{4}\right) = \frac{\left(-\frac{1}{2}\right)^{n+1}\left(-\frac{4097}{63}\right)}{3/2}$$

$$= (-1)^n\left(\frac{1}{2}\right)^{n+1}\left(\frac{8194}{189}\right).$$

The Single Hole

Consider a semi-infinite chain of springs and masses in which all the masses are the same and all the spring constants are the same except perhaps one of them (see Figure 12).

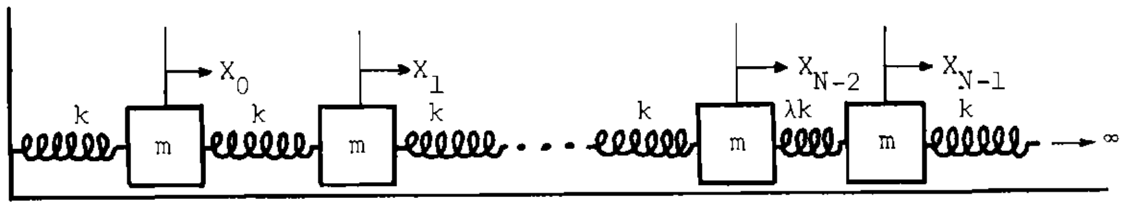


Figure 12. A Semi-Infinite Chain with a Single Hole

The case N = 1, for which the initial spring may be different from the others, should be interpreted differently from the other cases ($N \geq 2$), since the initial spring constant represents not a binding force between masses, but the binding force between a semi-infinite chain and the inertial system. If N = 1, recurrence (62) becomes

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_1(x) = 2x + \lambda - 1,$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad n\geq 1.$$

Hence,

$$R_1(x) = Q_1(x) + (\lambda-1)Q_0(x),$$

and

$$R_2(x) = Q_2(x) + (\lambda-1)Q_1(x).$$

So

$$R_n(x) = Q_n + (\lambda-1)Q_{n-1}(x), \quad n\geq 1,$$

and $P(z) = (\lambda-1)z + 1$. The zero of $P(z)$, for $\lambda \neq 1$, is $\frac{1}{1-\lambda}$, which is outside $(-1,0)$ if $0 < \lambda < 2$, is equal to -1 if $\lambda = 2$, is inside $(-1,0)$ if $\lambda > 2$, and is equal to 1 if $\lambda = 0$. The case $\lambda = 0$ is of particular interest, since it leads to a uniform chain which is not bound to an inertial system (see Chapter VI).

Now suppose that $N \geq 2$. The positive number λ and the integer N are treated as parameters. Recurrence (62) becomes

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad 0\leq n\leq N-3 \text{ and } n\geq N,$$

$$R_{N-1}(x) = \left[\frac{2}{\lambda} x + \left(1 - \frac{1}{\lambda}\right)\right] R_{N-2}(x) - \frac{1}{\lambda} R_{N-3}(x),$$

$$R_N(x) = [2x+(\lambda-1)]R_{N-1}(x) - \lambda R_{N-2}(x).$$

It is found that $R_n(x) = Q_n(x)$ for $0 \le n \le N-2$, that

$$R_{N-1}(x) = \frac{1}{\lambda} Q_{N-1}(x) + \left(1 - \frac{1}{\lambda}\right) Q_{N-2}(x),$$

and that

$$R_N(x) = \frac{1}{\lambda} Q_N(x) + 2\left(1 - \frac{1}{\lambda}\right) Q_{N-1}(x) - 2\left(1 - \frac{1}{\lambda}\right) Q_{N-2}(x) + \left(1 - \frac{1}{\lambda}\right) Q_{N-3}(x).$$

Identities (18) and (22) are then used to obtain

$$R_{2N}(x) = \frac{1}{\lambda} Q_{2N}(x) + 2\left(1 - \frac{1}{\lambda}\right) \sum_{\ell=1}^{N-1} [Q_{2\ell+1}(x)-Q_{2\ell}(x)] + \left(1 - \frac{1}{\lambda}\right) Q_1(x).$$

Hence,

$$P(z) = \left(1 - \frac{1}{\lambda}\right) z^{2N-1} + 2\left(1 - \frac{1}{\lambda}\right) \sum_{\ell=1}^{2N-2} (-1)^{\ell+1} z^{\ell} + \frac{1}{\lambda} .$$

The last equation can be written

$$P(z) = \left(1 - \frac{1}{\lambda}\right) g(z) + 1, \tag{77}$$

where

$$g(z) \overset{d}{=} z^{2N-1} + 2 \sum_{\ell=1}^{2N-2} (-1)^{\ell+1} z^{\ell} - 1 = (z-1) \sum_{\ell=0}^{2N-2} (-1)^{\ell} z^{\ell}.$$

After noting that $\lambda = 1$ gives the expected result, it is assumed that $\lambda \neq 1$. Now $g(z) < 0$ for $z < 0$. Hence Equation (77) implies that $P(z)$ has no zeros in $(-1,0)$ if $0 < \lambda < 1$. Moreover, g is continuous and strictly increasing on $(-\infty,0)$; $g(0) = -1$; and $g(z) \to -\infty$ as $z \to -\infty$. It follows that the condition $P(z) = 0$ defines z as a negative-valued, continuous, strictly increasing function of λ on $(1,\infty)$ such that $z \to -\infty$ as $\lambda \to 1^+$ and $z \to 0$ as $\lambda \to \infty$. These properties are illustrated by Figure 13.

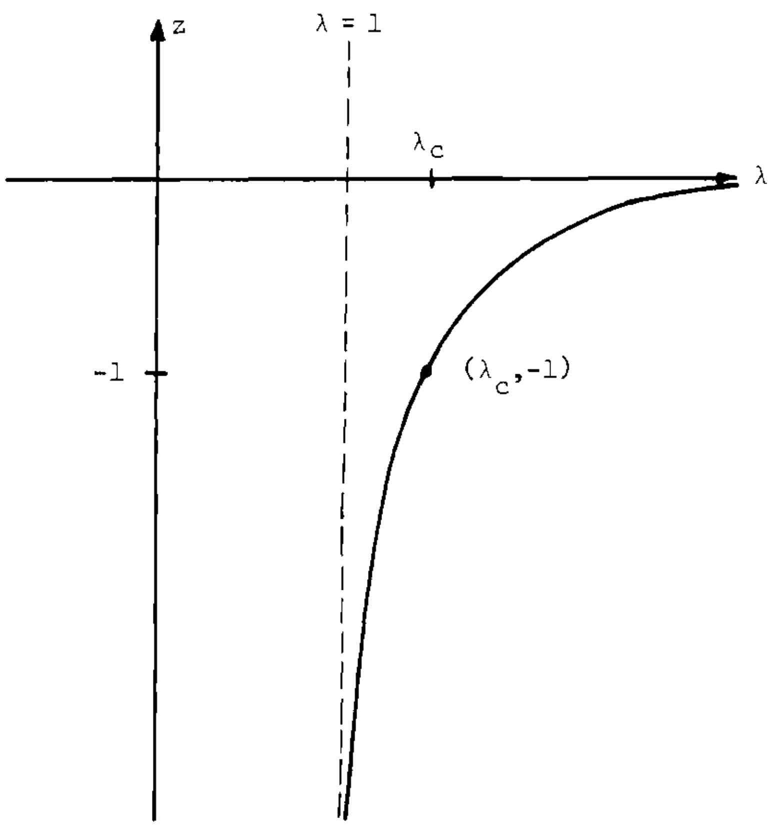


Figure 13. The Negative Real Zero of P(z) for the Single Hole

Hence, for $\lambda > 1$, $P(z)$ has exactly one zero in $(-\infty,0)$, and there is a "critical value" $\lambda_c \in (1,\infty)$, such that if $\lambda = \lambda_c$, $P(-1) = 0$. If $\lambda > \lambda_c$, $P(z)$ has one zero in $(-1,0)$; if $1 < \lambda < \lambda_c$, $P(z)$ has no zeros in $(-1,0)$. The number λ_c is determined by the condition $P(-1) = 0$:

$$\lambda_c = \frac{4N - 2}{4N - 3} .$$

Results for the single hole are given by the following summary. For fixed $N \geq 2$,

(i) if $0 < \lambda < \frac{4N - 2}{4N - 3}$ $(\lambda \neq 1)$, $P(z)$ has no zeros in $[-1,0)$; so $d\alpha_R(x)$ has support $[-1,1]$, and

$$d\alpha_R(x) = \frac{\frac{2}{\pi}(1-x^2)^{1/2}}{S(x)}\, dx;$$

(ii) if $\lambda = \frac{4N - 2}{4N - 3}$, $P(-1) = 0$ and $P(z)$ has no zeros in $(-1,0)$; so $d\alpha_R(x)$ has support $[-1,1]$, and

$$d\alpha_R(x) = \frac{\frac{1}{\pi}(1-x)^{1/2}(1+x)^{-1/2}}{S_2(x)}\, dx,$$

where $P(z) = (z+1)\hat{P}_2(z)$ and $S_2(x) = |\hat{P}_2(e^{i\theta})|^2$, $x = \cos\theta$;

(iii) if $\lambda > \frac{4N - 2}{4N - 3}$, $P(z)$ has exactly one zero, z_1, in $(-1,0)$; so $\alpha_R(x) = \alpha_1(x) + \alpha_2(x)$, where $d\alpha_1(x)$ has support $[-1,1]$,

$$d\alpha_1(x) = \frac{\frac{2}{\pi}(1-x^2)^{1/2}}{S(x)}\,dx,$$

and if $x_1 \overset{d}{=} \frac{1}{2}\left(z_1+z_1^{-1}\right)$,

$$d\alpha_2(x) = \frac{(z_1-z_1^{-1})^2}{z_1P(z_1^{-1})P'(z_1)}\;\delta(x-x_1)dx.$$

As in the case of the isotope, the determination of z_1 as an explicit function of λ and N seems presently unfeasible except perhaps in special cases.

The Single Interstitial

Consider a semi-infinite chain of springs and masses in which all the masses are the same except perhaps one of them. Also suppose that the spring constants of the two springs connected to the possibly perturbed mass are the same, but that this constant may be different from the common constant of the other springs (see Figure 14).

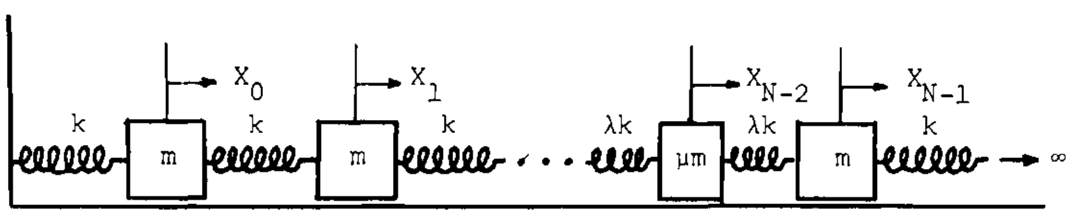


Figure 14. A Semi-Infinite Chain with a Single Interstitial

In order for the physical system to meet the requirements stated above, it is necessary that N be at least 2; moreover, since the case $N = 2$ involves a change in the initial spring constant (unless $\lambda = 1$, in which case the interstitial becomes an isotope--a case already discussed), the physical interpretation as an interstitial defect seems inappropriate when $N = 2$. Therefore, it is assumed that $N \geq 3$ in the succeeding discussion. The positive numbers μ and λ and the integer N are treated as parameters.

Recurrence (62) becomes

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad 0 \leq n \leq N-4 \text{ and } n \geq N,$$

$$R_{N-2}(x) = \left[\frac{2}{\lambda} x + \left(1 - \frac{1}{\lambda}\right)\right] R_{N-3}(x) - \frac{1}{\lambda} R_{N-4}(x),$$

$$R_{N-1}(x) = \left[2 \frac{\mu}{\lambda} x + 2\left(1 - \frac{\mu}{\lambda}\right)\right] R_{N-2}(x) - R_{N-3}(x),$$

$$R_N(x) = [2x+(\lambda-1)]R_{N-1}(x) - \lambda R_{N-2}(x).$$

The following results are obtained from the above recurrence.

$$R_n(x) = Q_n(x), \quad 0 \leq n \leq N-3,$$

$$R_{N-2}(x) = \frac{1}{\lambda} Q_{N-2}(x) + \left(1 - \frac{1}{\lambda}\right) Q_{N-3}(x),$$

$$R_{N-1}(x) = \frac{\mu}{\lambda^2} Q_{N-1}(x) + \left[-\frac{3\mu}{\lambda^2} + \frac{\mu}{\lambda} + \frac{2}{\lambda}\right] Q_{N-2}(x)$$

$$+ \left[\frac{3\mu}{\lambda^2} - \frac{2\mu}{\lambda} - \frac{2}{\lambda} + 1\right] Q_{N-3}(x) + \left[-\frac{\mu}{\lambda^2} + \frac{\mu}{\lambda}\right] Q_{N-4}(x),$$

$$R_N(x) = \frac{\mu}{\lambda^2} Q_N(x) + \left[-\frac{4\mu}{\lambda^2} + \frac{2\mu}{\lambda} + \frac{2}{\lambda}\right] Q_{N-1}(x)$$

$$+ \left[\frac{7\mu}{\lambda^2} - \frac{6\mu}{\lambda} - \frac{4}{\lambda} + \mu + 2\right] Q_{N-2}(x)$$

$$+ \left[-\frac{7\mu}{\lambda^2} + \frac{7\mu}{\lambda} + \frac{4}{\lambda} - 2\mu - 2\right] Q_{N-3}(x)$$

$$+ \left[\frac{4\mu}{\lambda^2} - \frac{4\mu}{\lambda} - \frac{2}{\lambda} + \mu + 1\right] Q_{N-4}(x) + \left[-\frac{\mu}{\lambda^2} + \frac{\mu}{\lambda}\right] Q_{N-5}(x),$$

where the equation for $R_N(x)$ is valid for $N \geq 4$ only. If $N = 3$,

$$R_3(x) = \frac{\mu}{\lambda^2} Q_3(x) + \left[-\frac{4\mu}{\lambda^2} + \frac{2\mu}{\lambda} + \frac{2}{\lambda}\right] Q_2(x)$$

$$+ \left[\frac{7\mu}{\lambda^2} - \frac{6\mu}{\lambda} - \frac{4}{\lambda} + \mu + 2\right] Q_1(x)$$

$$+ \left[-\frac{6\mu}{\lambda^2} + \frac{6\mu}{\lambda} + \frac{4}{\lambda} - 2\mu - 2\right] Q_0(x).$$

The above results together with identities (18) and (22) and rather tedious but routine calculations yield a formula for $R_{2N}(x)$, from which it is found that

$$P(z) = \left[\frac{\mu}{\lambda} - \frac{\mu}{\lambda^2}\right] z^{2N-1} + \left[\frac{4\mu}{\lambda^2} - \frac{4\mu}{\lambda} - \frac{2}{\lambda} + \mu + 1\right] z^{2N-2}$$

$$+ \left[-\frac{7\mu}{\lambda^2} + \frac{7\mu}{\lambda} + \frac{4}{\lambda} - 2\mu - 2\right] z^{2N-3}$$

$$+ \left[\frac{8\mu}{\lambda^2} - \frac{8\mu}{\lambda} - \frac{4}{\lambda} + 2\mu + 2\right] \sum_{\ell=3}^{2N-4} (-1)^{\ell} z^{\ell}$$

$$+ \left[\frac{7\mu}{\lambda^2} - \frac{6\mu}{\lambda} - \frac{4}{\lambda} + \mu + 2\right] z^2 + \left[-\frac{4\mu}{\lambda^2} + \frac{2\mu}{\lambda} + \frac{2}{\lambda}\right] z + \frac{\mu}{\lambda^2} .$$

In case N = 3, the sum $\sum_{\ell=3}^{2N-4} (-1)^{\ell} z^{\ell}$ is interpreted as *zero* in the above expression.

In the present case, the polynomial P(z) has not been analyzed to the extent that it was for the isotope and hole. However, upon examining the results for the isotope and hole, one might suspect that the relation between μ and λ defined by the equation P(-1) = 0 is somehow "critical" in determining the number of zeros of P(z) in (-1,0). The equation P(-1) = 0 yields, after some simplification,

$$\mu = -\frac{\lambda[(4N-7)\lambda-(8N-12)]}{4(\lambda-2)[(N-2)\lambda-(2N-3)]} . \tag{78}$$

The salient properties of this relation are illustrated in Figure 15.

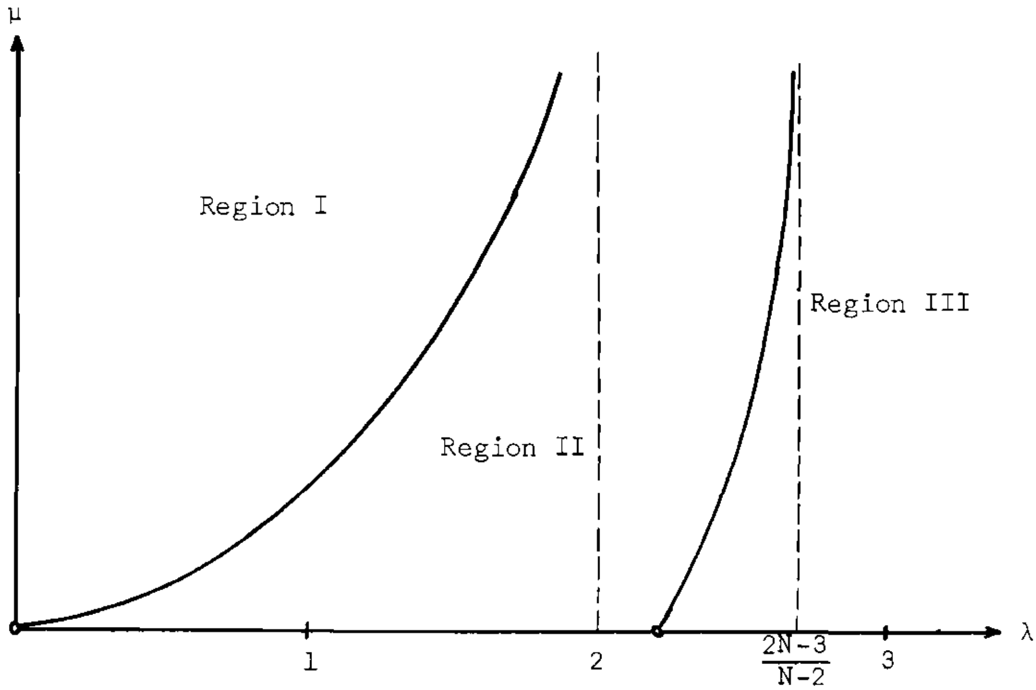


Figure 15. Relation Between μ and λ When P(-1) = 0 for the Single Interstitial

If (λ,μ) lies on one of the curves shown there, the corresponding P(z) has a zero at z = -1. If continuity of the zeros of P(z) as functions of (λ,μ) is assumed, then each of the three regions into which the graph of the "critical relation" divides the first quadrant of the λμ-plane might be conjectured to correspond to a fixed number of zeros of the associated P(z)'s in the interval (-1,0). If this is indeed the case, then from results for the isotope (λ=1) one infers that Region I corresponds to no zeros of P(z) in (-1,0) and that Region II corresponds to one zero of P(z) in (-1,0). These ideas and the possible significance of Region III are explored further in the examples which follow.

Suppose that $N \geq 3$ is arbitrary, $\mu > 0$ is arbitrary, and $\lambda = 2$.

Then

$$P(z) = \frac{\mu}{4} z^{2N-1} - \frac{\mu}{4} z^{2N-3} - \frac{\mu}{4} z^2 + z + \frac{\mu}{4} .$$

The condition $P(z) = 0$ leads to

$$\mu = \frac{-4z}{(z^{2N-3}-1)(z^2-1)} \overset{d}{=} g_1(z). \tag{79}$$

Now g_1 is continuous, positive-valued, and strictly decreasing on $(-1,0)$; moreover, $g_1(0) = 0$, and $g_1(z) \to +\infty$ as $z \to -1^+$. Hence (79) defines z as a continuous, strictly decreasing function of μ on $(0,\infty)$; and, for all $\mu > 0$, $z \in (-1,0)$ (see Figure 16).

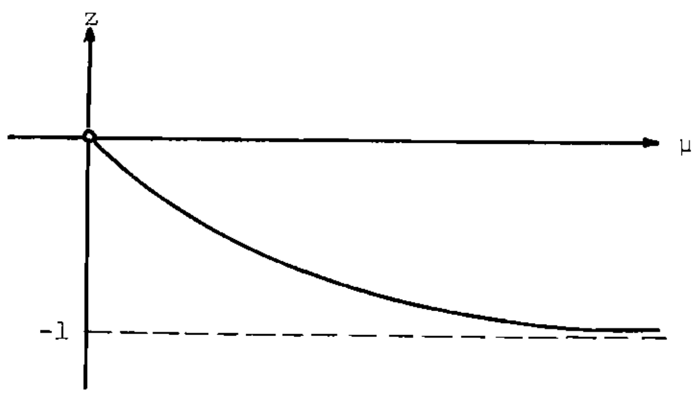


Figure 16. The Real Zero of P(z) for the Single Interstitial (λ=2)

By hypothesis, z is a zero of P(z). Hence, if $\lambda = 2$, P(z) has exactly one zero in $(-1,0)$ regardless of the values of N and μ (cf. Fig. 15). Thus, for the interstitial, the distribution function α_R always has a point of increase outside [-1,1] when $\lambda = 2$.

Another special case is now considered. Suppose that $N = 3$, $\lambda = 3$, and $\mu > 0$ is arbitrary. In this case,

$$P(z) = \frac{2}{9}\mu z^5 + \frac{1}{9}(\mu+3)z^4 - \frac{2}{9}(2\mu+3)z^3$$

$$- \frac{2}{9}(\mu-3)z^2 + \frac{2}{9}(\mu+3)z + \frac{1}{9}\mu .$$

The condition $P(z) = 0$ leads to

$$\mu = \frac{-3z(z^3-2z^2+2z+2)}{2\left(z + \frac{1}{2}\right)\left(z^2 - 1\right)^2} .$$

The important features of the above relation are shown in Figure 17.

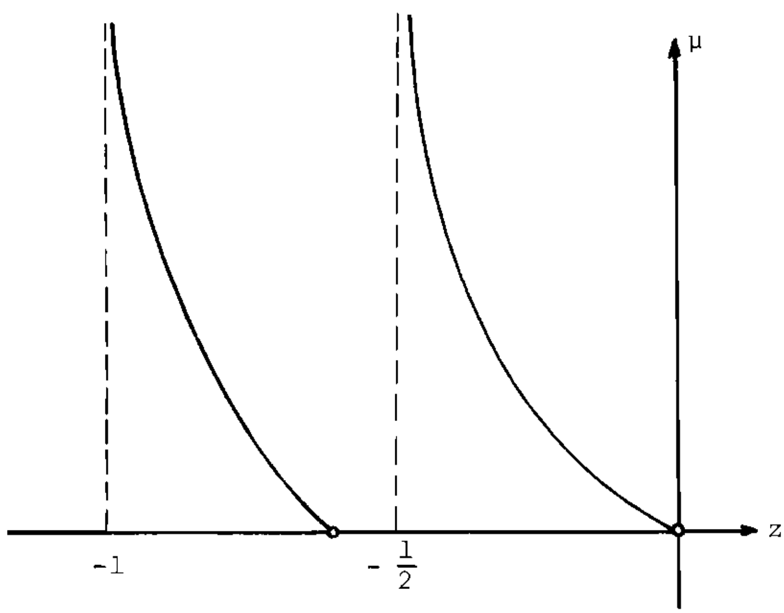


Figure 17. μ as a Function of the Real Zero of $P(z)$ in $(-1,0)$ for the Single Interstitial ($N=3$, $\lambda=3$)

It follows that, in this case, there are exactly *two* zeros of $P(z)$ in $(-1,0)$ for each $\mu > 0$ (which suggests that Region III (Fig. 15) may correspond to the cases in which $P(z)$ has exactly two zeros in $(-1,0)$). Thus, if $N = 3$ and $\lambda = 3$, the distribution function α_R has *two* points of increase outside $[-1,1]$.

CHAPTER VI

THE SINGLE ISOTOPE, HOLE, AND INTERSTITIAL IN THE CHAIN WITHOUT INITIAL SPRING

A semi-infinite chain of springs and masses in which the initial spring is not present--that is, a chain which is not bound to an inertial system--is a very important special case. It may be more attractive than the chain with initial spring as a physical model in the theory of lattice vibrations; and moreover, it plays a part in Martens' [15] solution of an initial-value problem for the symmetric fully infinite chain. In this chapter, the polynomial P(z) used to solve [IVP] for the semi-infinite chain with no initial spring is adduced for three cases: the chain with single isotope, the chain with single hole, and the chain with single interstitial. In addition, an example of a semi-infinite chain for which the associated distribution function α_R has two points of increase outside [-1,1] is given.

Consider a semi-infinite chain of springs and masses in which the initial spring constant is zero, the chain being uniform except for the presence of a single isotope (see Figure 18).

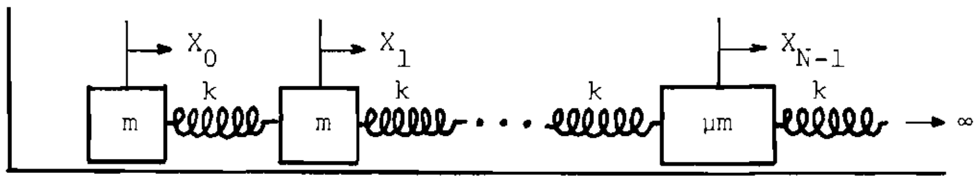


Figure 18. A Semi-Infinite Chain without Initial Spring and with a Single Isotope

Recurrence (62) becomes

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad 1 \le n \le N-2 \text{ and } n \ge N,$$

$$\left.\begin{aligned} R_1(x) &= 2x - 1, \\ R_N(x) &= \big(2\mu x + 2(1-\mu)\big)R_{N-1}(x) - R_{N-2}(x), \end{aligned}\right\} \text{ if } N \ge 2$$

$$R_1(x) = 2\mu x + (1-2\mu) = \mu Q_1(x) + (1-2\mu)Q_0(x), \quad \text{if } N=1.$$

For $N \ge 2$, the recurrence yields

$$R_n(x) = Q_n(x) - Q_{n-1}(x), \quad 0 \le n \le N-1,$$

$$R_N(x) = \mu Q_N(x) + (2-3\mu)Q_{N-1}(x) - 3(1-\mu)Q_{N-2}(x) + (1-\mu)Q_{N-3}(x).$$

The polynomial $R_{2N}(x)$ is determined in the usual way from the above information, and, for $N \ge 2$,

$$P(z) = (\mu-1)z^{2N} + 3(1-\mu)z^{2N-1} + 4(1-\mu) \sum_{\ell=2}^{2N-2} (-1)^{\ell+1} z^{\ell} + (2-3\mu)z + \mu.$$

For $N = 1$,

$$P(z) = (\mu-1)z^2 + (1-2\mu)z + \mu.$$

Now consider a semi-infinite chain of springs and masses in which the initial spring constant is zero, the chain being uniform except for the presence of a single hole (see Figure 19).

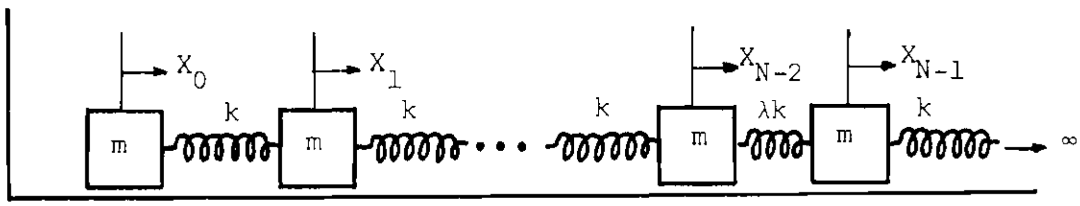


Figure 19. A Semi-Infinite Chain without Initial Spring and with a Single Hole

Necessarily $N \geq 2$ for such a system. Recurrence (62) becomes

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad 1 \leq n \leq N-3 \text{ and } n \geq N,$$

$$\left.\begin{aligned} R_1(x) &= 2x-1, \\ R_{N-1}(x) &= \left[\frac{2}{\lambda}x + \left(1 - \frac{1}{\lambda}\right)\right]R_{N-2}(x) - \frac{1}{\lambda}R_{N-3}(x), \end{aligned}\right\} \text{ if } N \geq 3$$

$$R_1(x) = \frac{2}{\lambda}x + \left(1 - \frac{2}{\lambda}\right), \quad \text{if } N=2,$$

$$R_N(x) = [2x+(\lambda-1)]R_{N-1}(x) - \lambda R_{N-2}(x).$$

From the recurrence, it is found that

$$R_n(x) = Q_n(x) - Q_{n-1}(x), \quad 0 \le n \le N-2,$$

$$R_{N-1}(x) = \frac{1}{\lambda} Q_{N-1}(x) + \left(1 - \frac{2}{\lambda}\right) Q_{N-2}(x) + \left(\frac{1}{\lambda} - 1\right) Q_{N-3}(x),$$

$$R_N(x) = \frac{1}{\lambda} Q_N(x) + \left(2 - \frac{3}{\lambda}\right) Q_{N-1}(x) + 4\left(\frac{1}{\lambda} - 1\right) Q_{N-2}(x)$$

$$+ 3\left(1 - \frac{1}{\lambda}\right) Q_{N-3}(x) + \left(\frac{1}{\lambda} - 1\right) Q_{N-4}(x), \quad \text{if } N \ge 3,$$

$$R_2(x) = \frac{1}{\lambda} Q_2(x) + \left(2 - \frac{3}{\lambda}\right) Q_1(x) + 3\left(\frac{1}{\lambda} - 1\right) Q_0(x), \quad \text{if } N=2.$$

These results lead to

$$P(z) = \left(1 - \frac{1}{\lambda}\right) z^{2N-1} - 3\left(1 - \frac{1}{\lambda}\right) z^{2N-2} + 4\left(1 - \frac{1}{\lambda}\right) \sum_{\ell=2}^{2N-3} (-1)^{\ell+1} z^{\ell}$$

$$+ \left(2 - \frac{3}{\lambda}\right) z + \frac{1}{\lambda},$$

where the sum $\sum_{\ell=2}^{2N-3} (-1)^{\ell+1} z^{\ell}$ is interpreted as zero if $N = 2$.

For a semi-infinite chain without initial spring into which a single interstitial has been introduced (see Figure 20), $N \ge 3$, necessarily; and recurrence (62) becomes

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad 1 \le n \le N-3 \text{ and } n \ge N,$$

$$\left.\begin{aligned} R_1(x) &= 2x - 1, \\ R_{N-2}(x) &= \left[\frac{2}{\lambda} x + \left(1 - \frac{1}{\lambda}\right)\right] R_{N-3}(x) - \frac{1}{\lambda} R_{N-4}(x), \end{aligned}\right\} N \ge 4$$

$$R_1(x) = \frac{2}{\lambda} x + \left(1 - \frac{2}{\lambda}\right), \quad N=3,$$

$$\left.\begin{aligned} R_{N-1}(x) &= \left[2 \frac{\mu}{\lambda} x + 2\left(1 - \frac{\mu}{\lambda}\right)\right] R_{N-2}(x) - R_{N-3}(x), \\ R_N(x) &= [2x + (\lambda-1)]R_{N-1}(x) - \lambda R_{N-2}(x). \end{aligned}\right\} N \ge 3$$

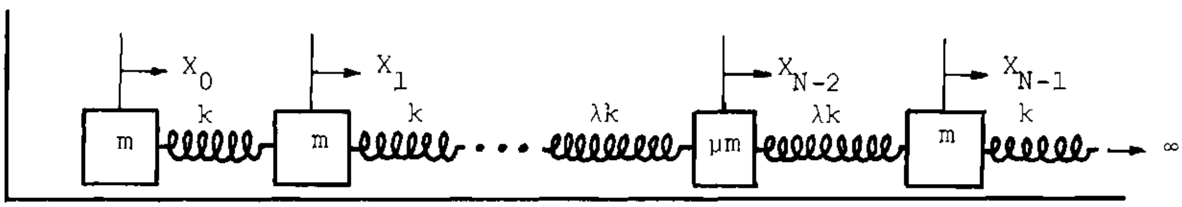


Figure 20. A Semi-Infinite Chain without Initial Spring and with a Single Interstitial

From the recurrence, it is found that

$$R_n(x) = Q_n(x) - Q_{n-1}(x), \quad 0 \le n \le N-3,$$

$$R_{N-2}(x) = \frac{1}{\lambda} Q_{N-2}(x) + \left(1 - \frac{2}{\lambda}\right) Q_{N-3}(x) + \left(\frac{1}{\lambda} - 1\right) Q_{N-4}(x), \quad N \ge 3,$$

$$R_{N-1}(x) = \frac{\mu}{\lambda^2} Q_{N-1}(x) + \left(-\frac{4\mu}{\lambda^2} + \frac{\mu}{\lambda} + \frac{2}{\lambda}\right) Q_{N-2}(x) + \left(\frac{6\mu}{\lambda^2} - \frac{3\mu}{\lambda} - \frac{4}{\lambda} + 1\right) Q_{N-3}(x)$$

$$+ \left(-\frac{4\mu}{\lambda^2} + \frac{3\mu}{\lambda} + \frac{2}{\lambda} - 1\right) Q_{N-4}(x) + \left(\frac{\mu}{\lambda^2} - \frac{\mu}{\lambda}\right) Q_{N-5}(x), \quad N\geq 4,$$

$$R_2(x) = \frac{\mu}{\lambda^2} Q_2(x) + \left(-\frac{4\mu}{\lambda^2} + \frac{\mu}{\lambda} + \frac{2}{\lambda}\right) Q_1(x) + \left(\frac{5\mu}{\lambda^2} - \frac{2\mu}{\lambda} - \frac{4}{\lambda} + 1\right) Q_0(x), \quad N=3,$$

$$R_N(x) = \frac{\mu}{\lambda^2} Q_N(x) + \left(-\frac{5\mu}{\lambda^2} + \frac{2\mu}{\lambda} + \frac{2}{\lambda}\right) Q_{N-1}(x) + \left(\frac{11\mu}{\lambda^2} - \frac{8\mu}{\lambda}\right.$$

$$\left. - \frac{6}{\lambda} + \mu + 2\right) Q_{N-2}(x) + \left(-\frac{14\mu}{\lambda^2} + \frac{13\mu}{\lambda} + \frac{8}{\lambda} - 3\mu - 4\right) Q_{N-3}(x)$$

$$+ \left(\frac{11\mu}{\lambda^2} - \frac{11\mu}{\lambda} - \frac{6}{\lambda} + 3\mu + 3\right) Q_{N-4}(x) + \left(-\frac{5\mu}{\lambda^2} + \frac{5\mu}{\lambda} + \frac{2}{\lambda}\right.$$

$$\left. - \mu - 1\right) Q_{N-5}(x) + \left(\frac{\mu}{\lambda^2} - \frac{\mu}{\lambda}\right) Q_{N-6}(x), \quad N\geq 5,$$

$$R_4(x) = \frac{\mu}{\lambda^2} Q_4(x) + \left(-\frac{5\mu}{\lambda^2} + \frac{2\mu}{\lambda} + \frac{2}{\lambda}\right) Q_3(x) + \left(\frac{11\mu}{\lambda^2} - \frac{8\mu}{\lambda} - \frac{6}{\lambda}\right.$$

$$\left. + \mu + 2\right) Q_2(x) + \left(-\frac{14\mu}{\lambda^2} + \frac{13\mu}{\lambda} + \frac{8}{\lambda} - 3\mu - 4\right) Q_1(x)$$

$$+ \left(\frac{10\mu}{\lambda^2} - \frac{10\mu}{\lambda} - \frac{6}{\lambda} + 3\mu + 3\right) Q_0(x), \quad N=4,$$

$$R_3(x) = \frac{\mu}{\lambda^2} Q_3(x) + \left(-\frac{5\mu}{\lambda^2} + \frac{2\mu}{\lambda} + \frac{2}{\lambda}\right) Q_2(x) + \left(\frac{10\mu}{\lambda^2} - \frac{7\mu}{\lambda}\right.$$

$$- \frac{6}{\lambda} + \mu + 2\Big) Q_1(x) + \left(- \frac{9\mu}{\lambda^2} + \frac{8\mu}{\lambda} + \frac{6}{\lambda} - 2\mu - 3\right) Q_0(x), \quad N=3.$$

These results lead to

$$P(z) = \left(- \frac{\mu}{\lambda^2} + \frac{\mu}{\lambda}\right) z^{2N-1} + \left(\frac{5\mu}{\lambda^2} - \frac{5\mu}{\lambda} - \frac{2}{\lambda} + \mu + 1\right) z^{2N-2} + \Big(- \frac{11\mu}{\lambda^2}$$

$$+ \frac{11\mu}{\lambda} + \frac{6}{\lambda} - 3\mu - 3\Big) z^{2N-3} + \left(\frac{15\mu}{\lambda^2} - \frac{15\mu}{\lambda} - \frac{8}{\lambda} + 4\mu + 4\right) z^{2N-4}$$

$$+ \left(\frac{16\mu}{\lambda^2} - \frac{16\mu}{\lambda} - \frac{8}{\lambda} + 4\mu + 4\right) \sum_{\ell=4}^{2N-5} (-1)^{\ell} z^{\ell} + \Big(- \frac{15\mu}{\lambda^2} + \frac{14\mu}{\lambda} + \frac{8}{\lambda}$$

$$- 3\mu - 4\Big) z^3 + \left(\frac{11\mu}{\lambda^2} - \frac{8\mu}{\lambda} - \frac{6}{\lambda} + \mu + 2\right) z^2 + \left(- \frac{5\mu}{\lambda^2} + \frac{2\mu}{\lambda} + \frac{2}{\lambda}\right) z$$

$$+ \frac{\mu}{\lambda^2}, \quad N \geq 4,$$

where $\sum_{\ell=4}^{2N-5} (-1)^{\ell} z^{\ell}$ is taken to be zero when $N = 4$;

$$P(z) = \left(- \frac{\mu}{\lambda^2} + \frac{\mu}{\lambda}\right) z^5 + \left(\frac{5\mu}{\lambda^2} - \frac{5\mu}{\lambda} - \frac{2}{\lambda} + \mu + 1\right) z^4$$

$$+ \left(- \frac{10\mu}{\lambda^2} + \frac{9\mu}{\lambda} + \frac{6}{\lambda} - 2\mu - 3\right) z^3 + \Big(\frac{10\mu}{\lambda^2} - \frac{7\mu}{\lambda} - \frac{6}{\lambda}$$

$$+ \mu + 2\Big) z^2 + \left(- \frac{5\mu}{\lambda^2} + \frac{2\mu}{\lambda} + \frac{2}{\lambda}\right) z + \frac{\mu}{\lambda^2}, \quad N=3.$$

It is observed that for all three cases considered above

$$P(z) = (z-1)\hat{P}_1(z),$$

where the following hold.

(i) For the isotope,

$$\hat{P}_1(z) = (\mu-1)z^{2N-1} + 2(1-\mu) \sum_{\ell=1}^{2N-2} (-1)^\ell z^\ell - \mu, \quad N\geq 1$$

(the sum $\sum_{\ell=1}^{2N-2} (-1)^\ell z^\ell$ is taken to be zero when $N = 1$).

(ii) For the hole,

$$\hat{P}_1(z) = \left(1 - \frac{1}{\lambda}\right)z^{2N-2} + 2\left(1 - \frac{1}{\lambda}\right) \sum_{\ell=1}^{2N-3} (-1)^\ell z^\ell - \frac{1}{\lambda}, \quad N\geq 2.$$

(iii) For the interstitial,

$$\hat{P}_1(z) = \left(- \frac{\mu}{\lambda^2} + \frac{\mu}{\lambda}\right)z^{2N-2} + \left(\frac{4\mu}{\lambda^2} - \frac{4\mu}{\lambda} - \frac{2}{\lambda} + \mu + 1\right)z^{2N-3}$$

$$+ \left(- \frac{7\mu}{\lambda^2} + \frac{7\mu}{\lambda} + \frac{4}{\lambda} - 2\mu - 2\right)z^{2N-4} + \left(\frac{8\mu}{\lambda^2}\right.$$

$$\left.- \frac{8\mu}{\lambda} - \frac{4}{\lambda} + 2\mu + 2\right) \sum_{\ell=3}^{2N-5} (-1)^\ell z^\ell + \left(- \frac{7\mu}{\lambda^2} + \frac{6\mu}{\lambda}\right.$$

$$+ \frac{4}{\lambda} - \mu - 2\Big)z^2 + \left(\frac{4\mu}{\lambda^2} - \frac{2\mu}{\lambda} - \frac{2}{\lambda}\right)z$$

$$- \frac{\mu}{\lambda^2}, \quad N\geq 5;$$

$$\hat{P}_1(z) = \left(- \frac{\mu}{\lambda^2} + \frac{\mu}{\lambda}\right)z^6 + \left(\frac{4\mu}{\lambda^2} - \frac{4\mu}{\lambda} - \frac{2}{\lambda} + \mu + 1\right)z^5$$

$$+ \left(- \frac{7\mu}{\lambda^2} + \frac{7\mu}{\lambda} + \frac{4}{\lambda} - 2\mu - 2\right)z^4 + \Big(\frac{8\mu}{\lambda^2} - \frac{8\mu}{\lambda} - \frac{4}{\lambda}$$

$$+ 2\mu + 2\Big)z^3 + \left(- \frac{7\mu}{\lambda^2} + \frac{6\mu}{\lambda} + \frac{4}{\lambda} - \mu - 2\right)z^2$$

$$+ \left(\frac{4\mu}{\lambda^2} - \frac{2\mu}{\lambda} - \frac{2}{\lambda}\right)z - \frac{\mu}{\lambda^2}, \quad N=4;$$

$$\hat{P}_1(z) = \left(- \frac{\mu}{\lambda^2} + \frac{\mu}{\lambda}\right)z^4 + \left(\frac{4\mu}{\lambda^2} - \frac{4\mu}{\lambda} - \frac{2}{\lambda} + \mu + 1\right)z^3$$

$$+ \left(- \frac{6\mu}{\lambda^2} + \frac{5\mu}{\lambda} + \frac{4}{\lambda} - \mu - 2\right)z^2 + \left(\frac{4\mu}{\lambda^2} - \frac{2\mu}{\lambda} - \frac{2}{\lambda}\right)z$$

$$- \frac{\mu}{\lambda^2}, \quad N=3.$$

It can be shown that if $P(z) = (z-1)\hat{P}_1(z)$ (where $\hat{P}_1(z) = \sum_{\ell=0}^{2N-1} \alpha_\ell z^\ell$, say), then for all $n \geq 2N-1$, $R_n(x) = - \sum_{\ell=0}^{2N-1} \alpha_\ell H_{n-\ell}(x)$. Thus in each of the above cases the polynomial $P(z)$ can be associated with the expansion of $R_n(x)$ $(n\geq 2N-1)$ in terms of the sequence $\{H_n(x)\}$. Moreover, in every case,

$$d\alpha_1(x) = \frac{w_1(x)}{S_1(x)}\,dx = \frac{1}{\pi}\,\frac{(1-x)^{-1/2}\,(1+x)^{1/2}}{S_1(x)}\,dx,$$

where $S_1(x) = |\hat{P}_1(e^{i\theta})|^2$. Points of increase of α_R outside $[-1,1]$ are determined by zeros of $\hat{P}_1(z)$ in $(-1,0)$.

As an example of a problem for which the distribution function α_R has more than one point of increase outside $[-1,1]$, consider the chain with two isotopes of equal mass depicted by Figure 21.

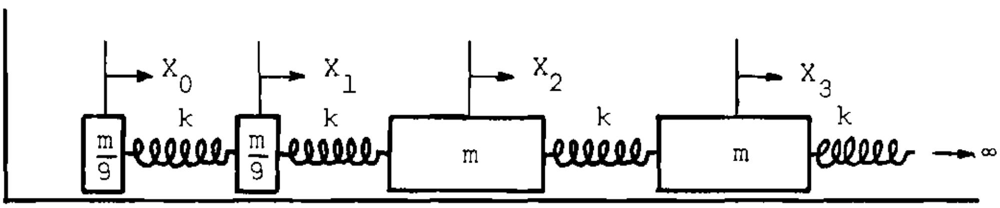


Figure 21. A Semi-Infinite Chain without Initial Spring and with Two Isotopes

The associated recurrence from (62) is

$$R_{-1}(x) = 0, \quad R_0(x) = 1,$$

$$R_1(x) = \frac{2}{9}\,x + \frac{7}{9}\,,$$

$$R_2(x) = \left(\frac{2}{9}\,x + \frac{16}{9}\right)R_1(x) - R_0(x),$$

$$R_{n+1}(x) = 2xR_n(x) - R_{n-1}(x), \quad n \geq 2.$$

For this example, N = 2, and it is found that

$$R_1(x) = \frac{1}{9} Q_1(x) + \frac{7}{9} Q_0(x),$$

$$R_2(x) = \frac{1}{81} Q_2(x) + \frac{23}{81} Q_1(x) + \frac{32}{81} Q_0(x),$$

$$R_3(x) = \frac{1}{81} Q_3(x) + \frac{23}{81} Q_2(x) + \frac{24}{81} Q_1(x) - \frac{40}{81} Q_0(x),$$

$$R_4(x) = \frac{1}{81} Q_4(x) + \frac{23}{81} Q_3(x) + \frac{24}{81} Q_2(x) - \frac{40}{81} Q_1(x) - \frac{8}{81} Q_0(x).$$

Thus,

$$P(z) = -\frac{1}{81} (8z^4 + 40z^3 - 24z^2 - 23z - 1)$$

$$= -\frac{1}{81} (z-1)(2z+1)(4z^2 + 22z + 1).$$

The zeros of P(z) are 1, $-\frac{1}{2}$, $\frac{1}{4}(-11 + 3\sqrt{13})$, and $\frac{1}{4}(-11 - 3\sqrt{13})$. Two of these zeros--

$$z_1 = \frac{1}{4}(-11 + 3\sqrt{13})$$

and

$$z_2 = -\frac{1}{2}$$

--are in (-1,0). The points of increase of α_R outside [-1,1] are, therefore,

$$x_1 = \frac{1}{2}(z_1+z_1^{-1}) = -\frac{1}{8}(55 + 9\sqrt{13}) \approx -10.9$$

and

$$x_2 = \frac{1}{2}(z_2+z_2^{-1}) = -\frac{5}{4}$$

(the corresponding frequencies are $\sqrt{\frac{2k}{m}(1-x_i)}$, $i=1,2$). The jumps $J(x_1)$ and $J(x_2)$ in α_R at x_1 and x_2 are

$$J(x_1) = \frac{(z_1-z_1^{-1})^2}{z_1 P(z_1^{-1})P'(z_1)} = \frac{5967 - 1071\sqrt{13}}{884} \approx 2.38$$

and

$$J(x_2) = 24.3.$$

Now $\alpha_R = \alpha_1 + \alpha_2$, where

$$d\alpha_1(x) = \frac{w_1(x)}{S_1(x)} = \frac{\frac{1}{\pi}(1-x)^{-1/2}(1+x)^{1/2}}{S_1(x)}\,dx$$

($S_1(x) = |\hat{P}_1(e^{i\theta})|^2$, where $\hat{P}_1(z) = -\frac{1}{81}(2z+1)(4z^2 + 22z + 1)$) and

$$d\alpha_2(x) = [J(x_1)\delta(x-x_1) + J(x_2)\delta(x-x_2)]dx$$

(see Figures 22 and 23).

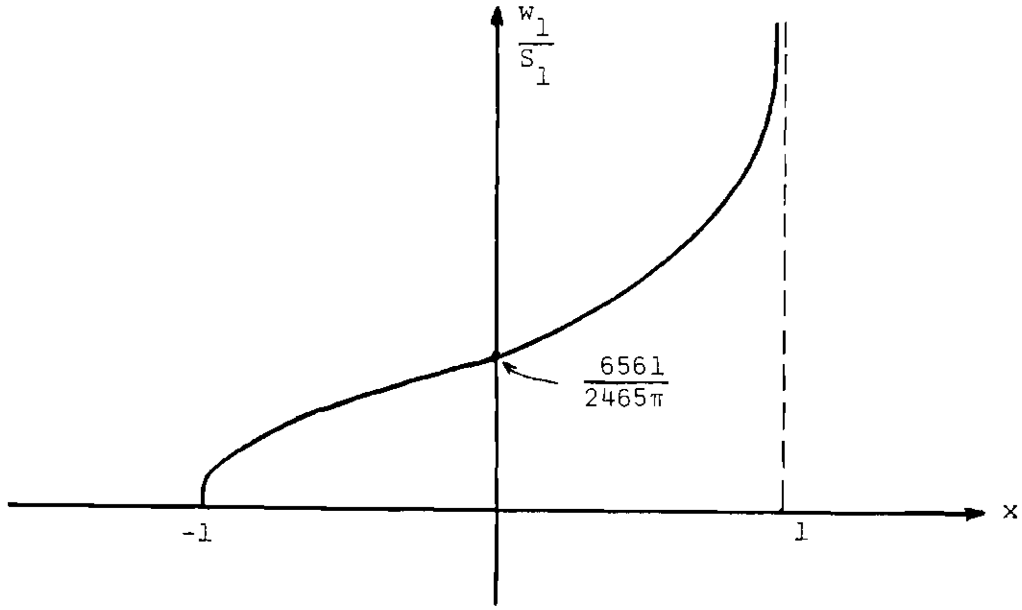


Figure 22. The Weight Function $\frac{w_1}{S_1}$

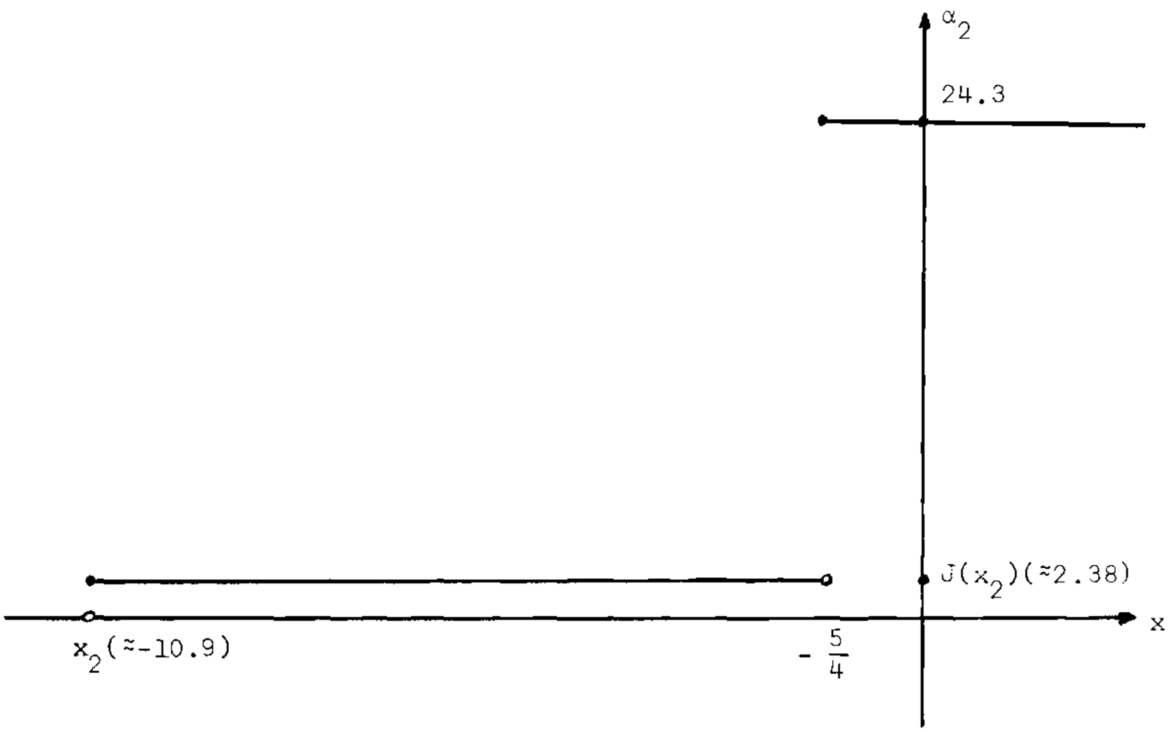


Figure 23. The Distribution Function α_2

APPENDIX

The purpose of this appendix is to show that if $\hat{z}$ is a zero of $P(z)$ and $-1 < \hat{z} < 1$ ($\hat{z} \neq 0$ by an earlier observation),

$$\hat{z}P'(\hat{z})P(\hat{z}^{-1}) > 0, \tag{A.1}$$

a result needed in the proof of Theorem 4.5. The nomenclature and results associated with the proof of Theorem 4.5 are used. In addition, it is helpful to have two results concerning the behavior of $R_n(x)$ and $R_n'(x)$ (for large n) near $\hat{x}$, a limit point of Z outside $[-1,1]$. These results (Lemmas A.2 and A.3) are established and then used to show (A.1).

For each $n \geq 1$, the polynomial $R_n(x)$ has n distinct, real zeros. These zeros are denoted by $x_{n,1}, x_{n,2}, \cdots, x_{n,n}$, where

$$x_{n,1} < x_{n,2} < \cdots < x_{n,n}.$$

Consider the sequences $\{x_{n,i}\}_{n=i}^{\infty}$ and $\{x_{n,n-j+1}\}_{n=j}^{\infty}$ for fixed $i, j \geq 1$--that is, the sequence obtained by recording the $(i-1)$*th*-from-smallest zero of each $R_n(x)$ $(n \geq i)$ and the sequence obtained by recording the $(j-1)$*th*-from-largest zero of each $R_n(x)$ $(n \geq j)$. By the interlacing property for the zeros of $\{R_n(x)\}$ these sequences are monotone. The following lemma shows that they are bounded.

Lemma A.1. The sequences $\{x_{n,1}\}_{n=1}^{\infty}$ and $\{x_{n,n}\}_{n=1}^{\infty}$ are bounded.

Proof. Suppose that $\{x_{n,1}\}$ is not bounded. Then by the monotonicity of this sequence,

$$\lim_{n\to\infty} x_{n,1} = -\infty. \tag{A.2}$$

It will be shown that this supposition leads to a contradiction.

By (A.2) there is an integer N_1 ($N_1 \geq 2N$) such that $x_{n,1} < -1$ for all $n \geq N_1$. Let $\tilde{z}_n = H^{-1}(x_{n,1})$ $(n \geq N_1)$. Then $-1 < \tilde{z}_n < 0$, and $R_n\left(H(\tilde{z}_n)\right) = R_n(x_{n,1}) = 0$ $(n \geq N_1)$; and furthermore, $\tilde{z}_n \uparrow 0$ as $n \to \infty$. Hence, by Equation (27),

$$0 = R_n\left(H(\tilde{z}_n)\right) = \frac{\tilde{z}_n^{n+1} P(\tilde{z}_n^{-1}) - \tilde{z}_n^{-(n+1)} P(\tilde{z}_n)}{\tilde{z}_n - \tilde{z}_n^{-1}}, \quad n \geq N_1.$$

It follows that

$$\tilde{z}_n^{n+1} P(\tilde{z}_n^{-1}) = \tilde{z}_n^{-(n+1)} P(\tilde{z}_n), \quad n \geq N_1. \tag{A.3}$$

Since $P(z)$ is a polynomial of degree at most $2N$ and since $|\tilde{z}_n| \leq |\tilde{z}_{N_1}| < 1$ for $n \geq N_1$,

$$\lim_{n\to\infty} \tilde{z}_n^{n+1} P(\tilde{z}_n^{-1}) = 0.$$

Hence, by (A.3)

$$\lim_{n\to\infty} \tilde{z}_n^{-(n+1)} P(\tilde{z}_n) = 0. \tag{A.4}$$

But $\lim_{n\to\infty} P(\tilde{z}_n) = P(0) \neq 0$ and $|\tilde{z}_n^{-(n+1)}| \to \infty$ as $n \to \infty$. So (A.4) cannot hold. Therefore, (A.2) is not possible. The proof that $\{x_{n,n}\}$ is bounded is similar. This concludes the proof.

Now let

$$\begin{aligned} \xi_i &= \lim_{n\to\infty} x_{n,i}, \qquad i\geq 1; \\ \eta_j &= \lim_{n\to\infty} x_{n,n-j+1}, \quad j\geq 1. \end{aligned} \tag{A.5}$$

Then $x_{n,i} \downarrow \xi_i$ and $x_{n,n-j+1} \uparrow \eta_j$ for each $i,j \geq 1$. Thus, ξ_i and η_j are limit points of Z. It follows, therefore, from Lemma 4.12 that whenever ξ_i or η_j is in the complement of $[-1,1]$, this number corresponds to a zero of $P(z)$ in $(-1,1)$. The lemma to be stated next shows that there is a one-to-one correspondence between the set of ξ_i and η_j in $(-\infty,-1) \cup (1,\infty)$ and the set of zeros of $P(z)$ in $(-1,1)$. Thus, each limit point of Z in $(-\infty,-1) \cup (1,\infty)$ can be identified with the limit of a special sequence of zeros of $\{R_n(x)\}$.

Lemma A.2. Suppose that $P(z)$ has zeros $z_1,\cdots,z_p$ in $(-1,1)$, and let q be the number of these zeros in $(-1,0)$. The nomenclature of Definition 4.4 is used, so that $-1 < z_1 < \cdots < z_q < 0$, if $q \neq 0$; and if $q \neq p$,

$0 < z_p < \cdots < z_{q+1} < 1$. Let ξ_i and η_j be defined by (A.5). Then

(i) $\xi_i \geq -1$ for $i \geq q+1$, and if $q > 0$,

$$\xi_i = H(z_i) \overset{d}{=} x_i, \quad 1 \leq i \leq q,$$

(ii) $\eta_j \leq 1$ for $j \geq p-q+1$, and if $p > q$,

$$\eta_j = H(z_{p-j+1}) \overset{d}{=} x_{p-j+1}, \quad 1 \leq j \leq p-q.$$

Proof. The proof of (i) will be given. The proof of (ii) is very similar.

Suppose that $q = 0$. Then, by Lemma 4.12, there are no limit points of Z in $(-\infty,-1)$. Since ξ_i $(i \geq 1)$ is a limit point of Z, it follows that $\xi_i \geq -1$ for all $i \geq 1$. The proof is complete in this case. Now suppose that $q \geq 1$. There are no elements of Z to the left of ξ_1, since $x_{n,1}$ is the smallest zero of $R_n(z)$ $(n \geq 1)$ and since $x_{n,1} \downarrow \xi_1$. Hence ξ_1 is the smallest limit point of Z. But this distinction also belongs to the number $H(z_1)$ by the way in which the z_j are ordered and by Lemma 4.12. Therefore, $\xi_1 = H(z_1)$. Thus, there is at least one element of $\{\xi_i: i \geq 1\}$ in $(-\infty,-1)$. Let K be the number of the ξ_i in $(-\infty,-1)$. Since ξ_1 is in $(-\infty,-1)$, $K > 0$. Moreover, since

$$\xi_1 \leq \xi_2 \leq \cdots ,$$

it must be the case that $\xi_i \in (-\infty,-1)$ $(1 \le i \le K)$ and $\xi_i \ge -1$ $(i > K)$. Since each ξ_i $(1 \le i \le K)$ is also a limit point of Z, and since $\{H(z_i): 1 \le i \le q\}$ is the set of *all* limit points of Z in $(-\infty,-1)$ (Lemma 4.12),

$$\{\xi_i: 1 \le i \le K\} \subset \{H(z_i): 1 \le i \le q\}.$$

If it is shown that the ξ_i $(1 \le i \le K)$ are *distinct* and that the reverse set inclusion holds, then (i) follows from the way in which these sets are ordered.

So suppose that $H(z_\ell) \notin \{\xi_i: 1 \le i \le K\}$ for some ℓ $(1 \le \ell \le q)$; in fact, with no loss in generality, it can be supposed that ℓ is the least positive integer with this property. The orderings of the ξ_i and $H(z_i)$ and the choice of ℓ imply that

$$\xi_K = H(z_{\ell-1}) < H(z_\ell).$$

Moreover,

$$\xi_{K+1} \ge -1 > H(z_\ell).$$

Let δ be small enough that the interval $\left(H(z_\ell)-\delta,\ H(z_\ell)+\delta\right)$ does not contain any element of $\{H(z_i): 1 \le i \le q\}$ except $H(z_\ell)$. From the preceding inequalities and since $x_{n,K} \downarrow \xi_K$ and $x_{n,K+1} \downarrow \xi_{K+1}$,

$$x_{n,K} < H(z_\ell)-\delta < H(z_\ell) < H(z_\ell)+\delta < x_{n,K+1}$$

for all n sufficiently large. Since $x_{n,K}$ and $x_{n,K+1}$ are consecutive zeros of $R_n(x)$, it follows that for all sufficiently large n there is no zero of $R_n(x)$ in $\left(H(z_\ell)-\delta,\ H(z_\ell)+\delta\right)$, which contradicts the fact that $H(z_\ell)$ is a limit point of Z. Therefore, $\{H(z_i)\colon 1\le i\le q\} \subset \{\xi_i\colon 1\le i\le K\}$; and so the two sets above are equal.

Now it will be shown that the ξ_i are distinct. If $K = 1$, the proof is complete. Suppose that $K > 1$ and that $\xi_s = \xi_{s+1}$ for some s: $1 \le s \le K-1$. Then, since $\{\xi_i\colon 1\le i\le K\} = \{H(z_i)\colon 1\le i\le q\}$,

$$\xi_s = \xi_{s+1} = H(z_t)$$

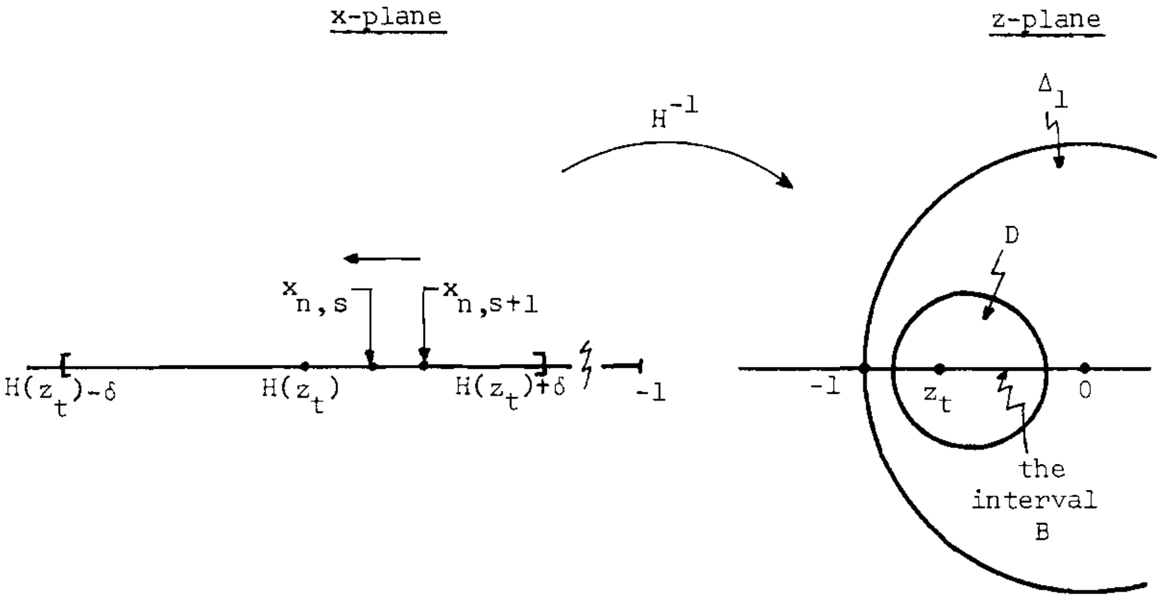
for some t ($1\le t\le q$). Hence, given $\delta > 0$, there is an integer $N_0 \ge 2N$ such that, for all $n \ge N_0$, there are at least two zeros of $R_n(x)$ in $\left(H(z_t)-\delta,\ H(z_t)+\delta\right)$--in particular, $x_{n,s}$ and $x_{n,s+1}$. It is assumed that $[H(z_t)-\delta,\ H(z_t)+\delta]$ is contained in $(-\infty,-1)$ and does not contain another $H(z_i)$. Let $B = H^{-1}\left[[H(z_t)-\delta,\ H(z_t)+\delta]\right]$. Then, by the properties of H, B is a closed interval, $B \subset (-1,0)$, and $z_t \in B$ (but z_t is not an end-point of B). Let D be the closed disk with center on the real axis and such that $D \cap (-1,0) = B$ (see figure on page 121). By the way D was constructed,

(i) $D \subset \Delta_1 - \{0\}$;

(ii) $z_t \in \text{int}(D)$;

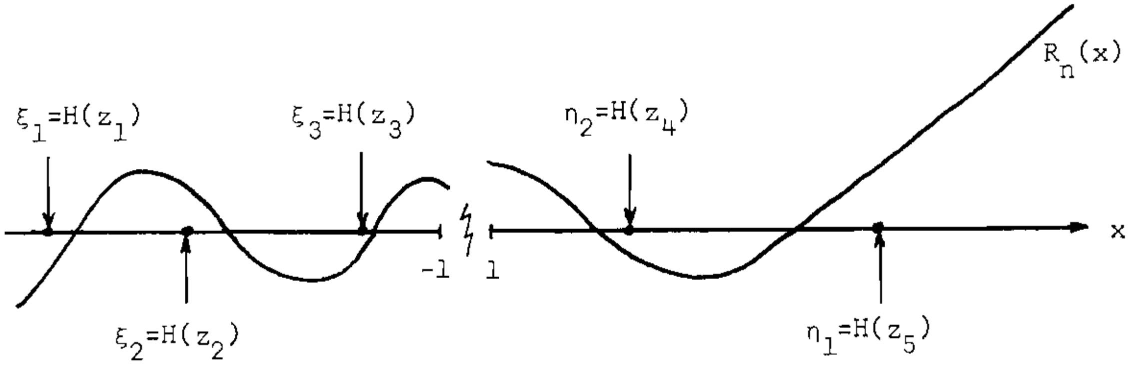
(iii) $P(z) \ne 0$ for $z \in D$, $z\ne z_t$;

(iv) for all $n \ge N_0$, $R_n\left(H(z)\right) = 0$ for at least two values of $z \in \text{int}(D)$.



As in the proof of Lemma 4.12, Rouché's Theorem can be applied to appropriately defined functions on D to conclude that P(z) has at least two zeros in the interior of D. But this conclusion, in turn, implies that z_t is a zero of P(z) of multiplicity at least 2, which contradicts Lemma 4.14. Therefore, the ξ_i are distinct. This concludes the proof.

It follows from the preceding lemma that the graph of R_n (for all sufficiently large n) has the qualitative appearance sketched on page 122 (p=5,q=3).



The location of the zeros of $R_n'(x)$ for x outside [-1,1] is now investigated. In particular, the proximity of these zeros to the limit points of Z outside [-1,1] is examined.

<u>Lemma A.3</u>. Let $\hat{x}$ be a limit point of Z, with $|\hat{x}| > 1$. Let I be any open interval containing $\hat{x}$, say $I = (\hat{x}-\delta_1,\ \hat{x}+\delta_2)$, where δ_1 and δ_2 are so chosen that $[\hat{x}-\delta_1,\ \hat{x}+\delta_2]$ contains no other limit point of Z in $(-\infty,-1) \cup (1,\infty)$ and $[\hat{x}-\delta_1,\ \hat{x}+\delta_2] \cap [-1,1] = \emptyset$. Then there exists an integer $N_1 \geq 2N$ such that for all $n \geq N_1$, $R_n'(\tilde{x}_n) = 0$ for *exactly one* $\tilde{x}_n \in I$.

<u>Proof</u>. Let $\hat{z} = H^{-1}(\hat{x})$. Then $P(\hat{z}) = 0$ by Lemma 4.12. Let D be the closed disk with center on the real axis and such that $D \cap (-1,1) = H^{-1}\left[[\hat{x}-\delta_1,\ \hat{x}+\delta_2]\right]$. From the properties of I it follows that

(i) $D \subset \Delta_1 - \{0\}$;

(ii) $\hat{z} \in \text{int}(D)$;

(iii) $P(z) \neq 0$ for $z \in D$, $z \neq \hat{z}$.

From (34)

$$R_n'\big(H(z)\big)H'(z)(z-z^{-1})^2 = (z-z^{-1})[-z^{n-1}P'(z^{-1}) + (n+1)z^nP(z^{-1})$$

$$- z^{-(n+1)}P'(z) + (n+1)z^{-(n+2)}P(z)]$$

$$- (1+z^{-2})[z^{n+1}P(z^{-1}) - z^{-(n+1)}P(z)], \quad n\geq 2N, \quad 0<|z|<1. \qquad (A.6)$$

Define γ_n, ρ_n, τ_n and σ_n, $n \geq 2N$, $0 < |z| < 1$, by

$$\gamma_n(z) = R_n'\big(H(z)\big)H'(z)(z-z^{-1})^2,$$

$$\rho_n(z) = (z-z^{-1})[-z^{n-1}P'(z^{-1}) + (n+1)z^nP(z^{-1})]$$

$$- (1+z^{-2})z^{n+1}P(z^{-1}),$$

$$\tau_n(z) = (z-z^{-1})[-z^{-(n+1)}P'(z)] + (1+z^{-2})z^{-(n+1)}P(z),$$

$$\sigma_n(z) = (z-z^{-1})(n+1)z^{-(n+2)}P(z).$$

These definitions and (A.6) yield

$$\gamma_n(z) = \rho_n(z) + \tau_n(z) + \sigma_n(z), \quad n\geq 2N, \quad 0<|z|<1. \qquad (A.7)$$

Estimates of these functions on ∂D are now determined. Thus, let $M = \max_{z\in\partial D} |z|$, and note that $0 < M < 1$. Now, for $z \in \partial D$ and $n \geq 2N$,

$$|\rho_n(z)| \le M^{n-1} \max_{z\varepsilon\partial D} \{|z-z^{-1}||P'(z^{-1})|\}$$

$$+ M^n \max_{z\varepsilon\partial D} \{|z-z^{-1}||P(z^{-1})|\}(n+1)$$

$$+ M^{n+1} \max_{z\varepsilon\partial D} \{|1+z^{-2}||P(z^{-1})|\}.$$

Hence, there exists an integer N_0 ($N_0 \ge 2N$) such that

$$|\rho_n(z)| < 1, \quad z\varepsilon\partial D, \quad n \ge N_0. \tag{A.8}$$

Let $C = \max_{z\varepsilon\partial D} \{|z-z^{-1}||P'(z)| + |1+z^{-2}||P(z)|\}$. Then

$$|\tau_n(z)| \le |z|^{-(n+1)}C, \quad z\varepsilon\partial D, \quad n \ge N_0. \tag{A.9}$$

Furthermore, if $m = \min_{z\varepsilon\partial D} \{|1-z^{-2}||P(z)|\}$, then $m > 0$, and

$$|\sigma_n(z)| \ge |z|^{-(n+1)}(n+1)m, \quad z\varepsilon\partial D, \quad n \ge N_0. \tag{A.10}$$

Now let $N_1 \ge N_0$ be chosen so that

$$M^{-(n+1)}[(n+1)m-C] > 1, \quad n \ge N_1$$

(such an N_1 exists since $0 < M < 1$ and $(n+1)m > C$ for all n large enough). Hence, for all $n \ge N_1$ and $z \varepsilon \partial D$, the preceding inequality yields

$$|z|^{-(n+1)}[(n+1)m-C] \geq M^{-(n+1)}[(n+1)m-C] > 1,$$

or

$$|z|^{-(n+1)}(n+1)m > |z|^{-(n+1)}C + 1, \quad n \geq N_1, \ z \varepsilon \partial D. \tag{A.11}$$

Therefore, from (A.9), (A.10), and (A.11), the following inequality holds for $n \geq N_1$ $(N_1 \geq N_0 \geq 2N)$ and $z \ \varepsilon \ \partial D$:

$$|\sigma_n(z)| \geq |z|^{-(n+1)}(n+1)m > |z|^{-(n+1)}C + 1 > |\tau_n(z)|$$

$$+ |\rho_n(z)| \geq |\tau_n(z) + \rho_n(z)|.$$

Hence, by Rouché's Theorem and (A.7), the functions σ_n and γ_n have the same number of zeros in the interior of D for each $n \geq N_1$. But $\gamma_n(z) = 0$ for some $z \ \varepsilon$ int(D) if and only if $R_n'\{H(z)\} = 0$, and $\sigma_n(z) = 0$ for some $z \ \varepsilon$ int(D) if and only if $P(z) = 0$. Therefore, $R_n'\{H(z)\}$ and $P(z)$ have the same number of zeros in int(D) for each $n \geq N_1$. Now $\hat{z}$ is the only zero of $P(z)$ in int(D), and $\hat{z}$ is a simple zero by Lemma 4.14. It follows that $R_n'\{H(z)\}$ has exactly one zero, say $\tilde{z}_n$, in int(D), for each $n \geq N_1$. Let $\tilde{x}_n = H(\tilde{z}_n)$. By the fact that the zeros of $R_n'(x)$ are real and by the way D was constructed, $\tilde{x}_n \ \varepsilon \ I$ $(n \geq N_1)$; moreover, $\tilde{x}_n$ is the only zero of $R_n'(x)$ in I, for each $n \geq N_1$. This completes the proof.

The preceding two lemmas are now used to establish the validity of (A.1).

<u>Proof (A.1)</u>. Suppose $P(\hat{z}) = 0$, where $0 < |\hat{z}| < 1$. Equation (34) yields $R_n'\left(H(\hat{z})\right)$ in the form

$$R_n'\left(H(\hat{z})\right) = F(n) - \frac{\hat{z}^{-(n+1)}\ P'(\hat{z})}{(\hat{z}-\hat{z}^{-1})H'(\hat{z})}\ ,\quad n\geq 2N,$$

where $F(n) \to 0$ as $n \to \infty$. The modulus of the second term in the preceding equation is bounded below by a positive constant. Hence, there is an integer N_0 $(N_0 \geq 2N)$ such that

$$\operatorname{sgn}\{R_n'\left(H(\hat{z})\right)\} = \operatorname{sgn}\left\{\frac{-\hat{z}^{-(n+1)}P'(\hat{z})}{(\hat{z}-\hat{z}^{-1})H'(\hat{z})}\right\},\quad n\geq N_0. \qquad (A.12)$$

Now $|\hat{z}| < 1$ implies that $\operatorname{sgn}(\hat{z}-\hat{z}^{-1}) = -\operatorname{sgn}\hat{z}$, and since $H'(\hat{z}) = \frac{1}{2}(1-\hat{z}^{-2})$, $\operatorname{sgn}\left(H'(\hat{z})\right) = -1$. Hence (A.12) can be reduced to

$$\operatorname{sgn}\{R_n'\left(H(\hat{z})\right)\} = -\operatorname{sgn}\{\hat{z}^{-n}P'(\hat{z})\},\quad n\geq N_0. \qquad (A.13)$$

Furthermore, from Equation (27),

$$R_n\left(H(\hat{z})\right) = \frac{\hat{z}^{n+1}\ P(\hat{z}^{-1})}{\hat{z}\ -\ \hat{z}^{-1}}\ ,\quad n\geq 2N.$$

Hence,

$$\operatorname{sgn}\{R_n(H(\hat{z}))\} = -\operatorname{sgn}\{\hat{z}^n\ P(\hat{z}^{-1})\}, \quad n \geq 2N. \tag{A.14}$$

Now let $\delta > 0$ be small enough so that the open intervals of radius δ about each of the limit points of Z in $(-\infty,-1) \cup (1,\infty)$ are mutually disjoint and none of these intervals intersects $[-1,1]$. $H(\hat{z})$ is one of these limit points. By Lemmas A.2 and A.3 and the fact that only finitely many constraints are involved, there exists an integer $N_1 \geq N_0$ such that the following hold for *each* of these limit points $(x_1,\cdots,x_p$, in the nomenclature of Definition 4.4):

(i) $R_n(x)$ has exactly one zero in the δ-interval (constructed above) about x_i for each $n \geq N_1$;

(ii) $R_n'(x)$ has exactly one zero in the δ-interval about x_i for each $n \geq N_1$.

In particular conditions (i) and (ii) hold for $\hat{x}$.

Consider (i) for $\hat{x}$. For each $n \geq N_1$, let $\bar{x}_n$ be the zero of $R_n(x)$ in $(\hat{x}-\delta,\hat{x}+\delta)$. If $\hat{x} < -1$, then $\bar{x}_n > \hat{x}$; if $\hat{x} > 1$, then $\bar{x}_n < \hat{x}$ (see figure below).

$(\hat{x}<-1)$ $(\hat{x}>1)$

There are no zeros of $R_n(x)$ between $\hat{x}$ and $\bar{x}_n$ for $n \geq N_1$. Moreover,

$R_n'(\bar{x}_n) \neq 0$, since the zeros of $R_n(x)$ are simple; and $R_n(\hat{x}) \neq 0$ $(n \geq N_1)$ since the simultaneous assumption that $R_n(\hat{x}) = 0$ leads to a contradiction (as in the proof of Lemma 4.12). The possibilities for sgn $R_n(\hat{x})$ and $\operatorname{sgn}[R_n'(\bar{x}_n)]$ may be summarized as follows.

$\underline{\hat{x} < -1}$	$\underline{\hat{x} > 1}$
If $R_n(\hat{x}) > 0$, $R_n'(\bar{x}_n) < 0$.	If $R_n(\hat{x}) > 0$, $R_n'(\bar{x}_n) > 0$.
If $R_n(\hat{x}) < 0$, $R_n'(\bar{x}_n) > 0$.	If $R_n(\hat{x}) < 0$, $R_n'(\bar{x}_n) < 0$.

This table is represented by the equation

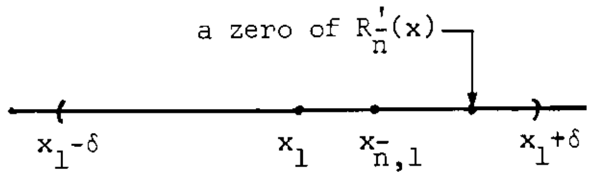
$$\operatorname{sgn}\{R_n'(\bar{x}_n)\} = \operatorname{sgn}\{\hat{x}R_n(\hat{x})\}, \quad n \geq N_1;$$

or, since sgn $\hat{x}$ = sgn $\hat{z}$ and since $\hat{x} = H(\hat{z})$,

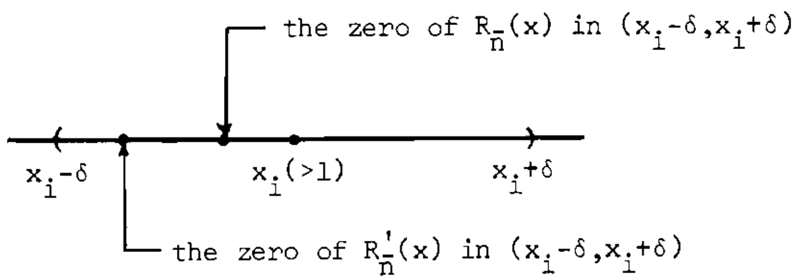
$$\operatorname{sgn}\{R_n'(\bar{x}_n)\} = \operatorname{sgn}\{\hat{z}R_n\big(H(\hat{z})\big)\}, \quad n \geq N_1. \tag{A.15}$$

Now consider condition (ii) for $\hat{x}$. Let $\tilde{x}_n$ be the zero of $R_n'(x)$ in $(\hat{x}-\delta, \hat{x}+\delta)$, $n \geq N_1$. It will be shown that for all $n \geq N_1$ $\tilde{x}_n$ does not lie between $\hat{x}$ and $\bar{x}_n$. Thus, let p denote the number of zeros of $P(z)$ in $(-1,1)$. For fixed (but arbitrary) $\bar{n} \geq N_1$, there are exactly p zeros of $R_{\bar{n}}(x)$ outside $[-1,1]$; and, by condition (ii), these zeros are located in the δ-intervals about x_i $(1 \leq i \leq p)$ (nomenclature of Theorem 4.14). Suppose that $x_1 < -1$ (i.e., suppose that there are limit points of Z in $(-\infty,-1)$). The zero of $R_{\bar{n}}(x)$ in $(x_1-\delta, x_1+\delta)$ is $x_{\bar{n},1}$, the smallest zero of $R_{\bar{n}}(x)$.

There are no zeros of $R'_{\bar{n}}(x)$ to the left of $x_{\bar{n},1}$. But there is exactly one zero of $R'_{\bar{n}}(x)$ in $(x_1-\delta, x_1+\delta)$ by condition (ii). Therefore, this zero must be in the interval $(x_{\bar{n},1}, x_1+\delta)$ (see figure below).

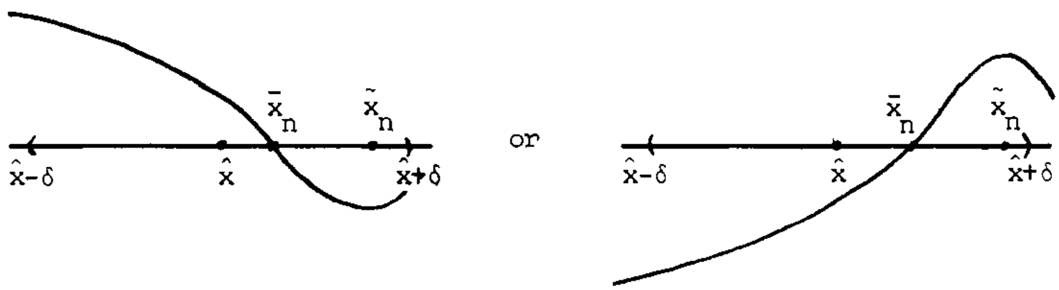


This accounts for the *one* zero of $R'_{\bar{n}}(x)$ between $x_{\bar{n},1}$ and $x_{\bar{n},2}$. Hence, the next zero of $R_{\bar{n}}(x)$ must lie to the right of $x_{\bar{n},2}$. Continuing in this manner until q (the number of limit points of Z in $(-\infty,-1)$) of the zeros of $R'_{\bar{n}}(x)$ are accounted for, it is seen that for each i $(1 \le i \le q)$, the zero of $R'_{\bar{n}}(x)$ in $(x_i-\delta, x_i+\delta)$ lies in the interval $(x_{\bar{n},i}, x_i+\delta)$. If there are no limit points of Z in $(1,\infty)$ the proof is complete. Otherwise, consider x_p, the largest such limit point. The zero of $R_{\bar{n}}(x)$ in $(x_p-\delta, x_p+\delta)$ is $x_{\bar{n},\bar{n}}$, the largest zero of $R_{\bar{n}}(x)$. There are no zeros of $R'_{\bar{n}}(x)$ to the right of $x_{\bar{n},\bar{n}}$, etc. By an argument completely symmetric to the one above, p - q of the zeros of $R'_{\bar{n}}(x)$ are accounted for; and for each i $(q+1 \le i \le p)$, the zero of $R'_{\bar{n}}(x)$ in $(x_i-\delta, x_i+\delta)$ is between $x_i - \delta$ and the zero of $R_{\bar{n}}(x)$ in this interval (see figure below).



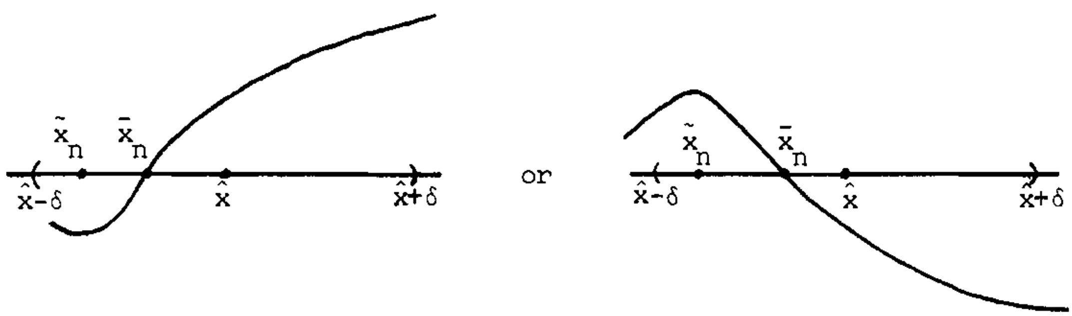
Thus, *all* the zeros of $R'_{\bar{n}}(x)$ are accounted for. But $\bar{n} \geq N_1$ was arbitrary. Thus for all $n \geq N_1$ it is seen that $\tilde{x}_n$ does not lie between $\hat{x}$ and $\bar{x}_n$.

The results in the last two paragraphs show that over the interval $(\hat{x}-\delta,\hat{x}+\delta)$ the graphs of R_n $(n \geq N_1)$ have the qualitative appearance sketched below.



$(\hat{x}<-1)$

or



$(\hat{x}>1)$

In particular, the fact that $\tilde{x}_n$ does not lie between $\hat{x}$ and $\bar{x}_n$ shows that

$$\operatorname{sgn}\{R_n'(\bar{x}_n)\} = \operatorname{sgn}\{R_n'(\hat{x})\}, \quad n \geq N_1,$$

or

$$\operatorname{sgn}\{R_n'(\bar{x}_n)\} = \operatorname{sgn}\{R_n'\big(H(\hat{z})\big)\}, \quad n \geq N_1. \tag{A.16}$$

Now $N_1 \geq N_0 \geq 2N$. So, by (A.13) - (A.16),

$$\begin{aligned}
-\operatorname{sgn}\{\hat{z}^{-n} P'(\hat{z})\} &= \operatorname{sgn}\{R_n'\big(H(\hat{z})\big)\} \\
&= \operatorname{sgn}\{R_n'(\bar{x}_n)\} \\
&= \operatorname{sgn}\{\hat{z}R_n\big(H(\hat{z})\big)\} \\
&= -\operatorname{sgn}\{\hat{z}^{n+1} P(\hat{z}^{-1})\}, \quad n \geq N_1.
\end{aligned}$$

Neither $\hat{z}^{-n} P'(\hat{z})$ nor $\hat{z}^{n+1} P(\hat{z}^{-1})$ is 0, because $\hat{z} \neq 0$, the zeros of $P(z)$ in $(-1,1)$ are simple, and $P(\hat{z}^{-1}) \neq 0$ (Lemma 4.16). Hence $0 < \hat{z}^{n+1} P(\hat{z}^{-1})\hat{z}^{-n} P'(\hat{z}) = \hat{z}P'(\hat{z})P(\hat{z}^{-1})$. This concludes the proof.

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VITA

William Pullin McKibben was born August 2, 1940, in Atlanta, Georgia. He completed his primary and secondary education in the public schools in McDonough, Georgia, and entered the Georgia Institute of Technology as a freshman in September, 1957, after completing his junior year of high school. He received the degree of Bachelor of Science in Applied Mathematics in June, 1961, and became a graduate student in applied mathematics in September, 1961. He served as a graduate teaching assistant in mathematics during the school years 1961-62 and 1962-63, and received the degree of Master of Science in Applied Mathematics in June, 1963.

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He is married to the former Valerie Trent Jackson of McDonough, Georgia. The McKibbens have one child, James Harkness McKibben, born August 8, 1967.